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Upscaling of an isothermal Li-ion battery model via the Homogenization Theory

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# Vorwort

Das Tätigkeitsfeld des Fraunhofer-Instituts für Techno- und Wirtschaftsmathematik ITWM umfasst anwendungsnahe Grundlagenforschung, angewandte Forschung sowie Beratung und kundenspezifische Lösungen auf allen Gebieten, die für Techno- und Wirtschaftsmathematik bedeutsam sind.

In der Reihe »Berichte des Fraunhofer ITWM« soll die Arbeit des Instituts kontinuierlich einer interessierten Öffentlichkeit in Industrie, Wirtschaft und Wissenschaft vorgestellt werden. Durch die enge Verzahnung mit dem Fachbereich Mathematik der Universität Kaiserslautern sowie durch zahlreiche Kooperationen mit internationalen Institutionen und Hochschulen in den Bereichen Ausbildung und Forschung ist ein großes Potenzial für Forschungsberichte vorhanden. In die Berichtreihe werden sowohl hervorragende Diplom- und Projektarbeiten und Dissertationen als auch Forschungsberichte der Institutsmitarbeiter und Institutsgäste zu aktuellen Fragen der Techno- und Wirtschaftsmathematik aufgenommen.

Darüber hinaus bietet die Reihe ein Forum für die Berichterstattung über die zahlreichen Kooperationsprojekte des Instituts mit Partnern aus Industrie und Wirtschaft.

Berichterstattung heißt hier Dokumentation des Transfers aktueller Ergebnisse aus mathematischer Forschungs- und Entwicklungsarbeit in industrielle Anwendungen und Softwareprodukte – und umgekehrt, denn Probleme der Praxis generieren neue interessante mathematische Fragestellungen.



Prof. Dr. Dieter Prätzel-Wolters  
Institutsleiter

Kaiserslautern, im Juni 2001



# Upscaling of an Isothermal Li-ion Battery Model via the Homogenization Theory

Y. Efendiev\*, O. Iliev<sup>†</sup>, V. Taralova<sup>†‡</sup>

## Abstract

Li-ion batteries are one of the most popular types of rechargeable batteries for portable electronics. They are multiscale systems with processes occurring at different scales. The aim of the mathematical modelling is better understanding of the electrochemical processes in Li-ion batteries as well as prolonging the batteries' lifetime and improving their performance. A broad range of scientific and engineering problems involve multiple scales. Direct numerical simulations lead to a huge number of degrees of freedom difficult to handle even with supercomputers. From an application perspective it is often sufficient to predict the macroscopic properties of the multiscale systems. The goal of the upscaling techniques for Lithium-ion battery models is to develop a method that captures the small-scale effects on the large scales, but does not require resolving all the small-scale features.

**Keywords:** Li-ion Batteries, Homogenization

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## List of Symbols

$c^e$  - concentration of lithium ions in the electrolyte

$c^s$  - concentration of lithium ions in the active particles

$\phi^e$  - potential in the electrolyte

$\phi^s$  - potential in the solid

$T$  - temperature

$D^e$  - interdiffusion coefficient in the electrolyte; strictly positive

$D^s$  - interdiffusion coefficient in the active particles; strictly positive

$t_+$  - transference number of Li ions

$\kappa^s$  - electric conductivity; strictly positive

$\mathbf{N}$  - ionic flux

$\mathbf{j}$  - electrical current

$F$  - Faraday constant

$R$  - Universal gas constant

$\eta_s$  - overpotential

$U_0$  - half cell open circuit potential

$c_{s,max}$  - maximum concentration of ions in the active particle

$k$  - reaction rate

$soc$  - state of charge, i.e.  $\frac{c_s}{c_{s,max}}$

# 1 Introduction

In this work we derive rigorously upscaled Li-ion battery model via the homogenization theory. We start from the microscopic model developed in [8]. Here we describe briefly the main components and processes in the battery. A more detailed description of the battery and the electrochemical processes involved is given in [12].

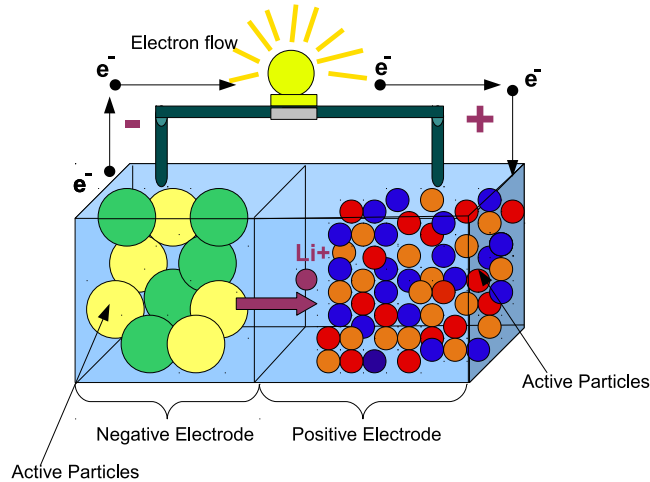


Figure 1: Battery Cell

A typical Li-ion battery consists of many electrically connected electrochemical cells. Each cell has two electrodes- anode and cathode, separator and electrolyte. The anode and the cathode have porous structure consisting of an active particle skeleton filled with liquid electrolyte (see Figure 1). During charge and discharge of the battery the lithium ions move from one electrode to the other. The model [8] is based on nonlinear diffusion equations for the transport of Lithium ions and charges in the electrolyte and in the active particles as well as their coupling due to electrochemical reactions on the interface boundary between the particles and the electrolyte. Usually in Li-ion batteries the number of particles in each electrode is very large. Resolving such a big number of particles in the microscale simulations would be very computationally expensive. The aim of the homogenization of the model is to derive equations on the macroscale which correctly capture the macroscopic behaviour of the battery cell without fully resolving all the microscopic features. This reduces significantly the computational cost. We consider periodically arranged active particles and we derive coupled micro-macroscopic model.

Another paper where homogenization of microscale Li-ion battery model is considered is [6]. However our approach differs in several aspects. First of all, they start from a different microscopic model [7]. Nevertheless, the two models are similar enough so that the approaches can be compared. In [6] it is stated that the current density is of the order of the small parameter but there is no justification. In the current work we derive this estimate mathematically. Another point is that the final homogenized model in [7] does not depend explicitly on the small parameter although it is present in the derivation. Furthermore it is not clear what boundary conditions are used in their model. In our case the boundary conditions are specified beforehand in the microscale setting of the model and they are homogenized along with the other equations. Finally we perform detailed numerical simulations in order to verify the proposed homogenization approach.

In the paper [9] the authors also apply the homogenization theory to derive macroscopic battery model. Their approach is very similar to ours. The differences are that they start

from a different microscopic model and do not provide a detailed numerical investigation in order to test their homogenized model against full microscopic simulations. In our work we run a series of numerical experiments varying the particles' size and we show a very good agreement between the solution of the homogenized model and that of the full microscopic model.

One of the most used models for Li-ion batteries on the scale of our homogenized problem is the model proposed by Newman et. al [5]. This model, however, is derived directly on the macroscale and is restricted only to spherical active particles, whereas our method allows for randomly shaped particles.

Our homogenization approach is also similar in some aspects to the one used by Arbogast et. al in [1, 2].

## 2 The Homogenization Method

The homogenization method [3], [10], [4] deals with partial differential equations with periodically oscillating coefficients. These type of equations model various physical problems arising in media with periodic structure. The aim of the method is to derive macroscale "homogenized" equations which adequately describe the macroscopic behaviour of the solution and in the same time significantly decrease the degrees of freedom of the considered problem. In these problems the size  $l$  of the periodic micro structure is small compared to the size  $L$  of a sample of the medium. We start from the microscopic description of the problem and we seek a macroscopic, or averaged, description.

Let us consider the following equation

$$\mathcal{L}u = f, \quad x \in \Omega \quad (2.1)$$

where  $\mathcal{L}$  is some partial differential operator and  $u$  and  $f$  are functions of  $x$ . We want to investigate the behaviour of the partial differential equation as  $\varepsilon = \frac{l}{L} \rightarrow 0$ , i.e. as the size of the periodicities  $l$  goes to zero which is equivalent to their number becoming infinitely large. Therefore an asymptotic analysis is required as  $\varepsilon \rightarrow 0$ . We obtain a family of partial differential operators  $\mathcal{L}_\varepsilon$  (with coefficients oscillating with period  $\varepsilon L$ ), and a family of solutions  $u_\varepsilon$ , which satisfy

$$\mathcal{L}_\varepsilon u_\varepsilon = f, \quad x \in \Omega \quad (2.2)$$

complemented by appropriate boundary conditions. Assuming that the sequence  $u_\varepsilon$  converges, in some sense, to a limit  $u^h$ , we look for a so-called homogenized operator  $\mathcal{L}^h$  such that  $u^h$  is a solution of

$$\mathcal{L}^h u^h = f, \quad x \in \Omega \quad (2.3)$$

We use the well-known two-scale asymptotic expansion method in order to find the precise form of the homogenized operator  $\mathcal{L}^h$ . We postulate the following ansatz for  $u_\varepsilon$

$$u_\varepsilon(x) = u_0\left(x, \frac{x}{\varepsilon}\right) + \varepsilon u_1\left(x, \frac{x}{\varepsilon}\right) + \varepsilon^2 u_2\left(x, \frac{x}{\varepsilon}\right) + \dots \quad (2.4)$$

where we denote

$$y = \frac{x}{\varepsilon} \quad (2.5)$$

and each term  $u_i(x, y)$  is periodic in  $y$ . Inserting the asymptotic expansion (2.4) in (2.2) and identifying equal powers of  $\varepsilon$  leads to a cascade of equations for each term  $u_i$ . Averaging with respect to  $y$  the equation for  $u_0$  gives the homogenized equation

$$\mathcal{L}^h u_0 = f \quad (2.6)$$

The precise form of the operator  $\mathcal{L}^h$  is computed with the help of a so-called auxiliary cell problem in the unit period. It is proved (see [3], [10], [4]) for linear elliptic problems that  $u_\varepsilon \rightarrow u_0$  in  $H^1(\Omega)$  weakly.

## 2.1 One Example: Two-Dimensional Linear Elliptic Problem

We consider the following linear elliptic equation with oscillating coefficient  $a_\varepsilon(x)$  ( $a_\varepsilon(x) > 0$  for  $\forall x \in \Omega$ , ellipticity condition), with period of the oscillations  $\varepsilon L$ :

$$-\nabla \cdot (a_\varepsilon(x) \nabla u_\varepsilon) = f(x), \quad x \in \Omega \subset \mathbb{R}^2 \quad (2.7a)$$

$$u_\varepsilon(x) = 0, \quad x \in \partial\Omega \quad (2.7b)$$

We assume that we have a regular periodic microstructure of the domain  $\Omega$  with  $\varepsilon L = l \ll L$  being the size of the periodicities. The medium varies rapidly on the small scale  $l$  and may also vary slowly on the large scale  $L$ . Here  $x$  is the so called global variable and  $y = \frac{x}{\varepsilon}$  is its respective local variable. Let us denote with  $\varepsilon Y_i$  the microscopic periodicity cells. Then after the change of variables  $y = \frac{x}{\varepsilon}$ , each microscopic periodicity cell  $\varepsilon Y_i$  with characteristic length  $l$  transforms into the upscaled periodicity cell  $Y_i$  with characteristic length  $L$ . Then we translate each cell  $Y_i$  into a reference periodicity cell  $Y$  via the translation  $\tau_i$ :

$$\tau_i : y' = y + \xi_i \quad (2.8)$$

where  $\xi_i$  is a given constant vector for each cell  $Y_i$ . It is clear that the characteristic length of the reference periodicity cell  $Y$  is also  $L$ . From now on, unless specified otherwise, we will say that a function  $g(x, y)$  is  $Y$ -periodic in the  $y$  variable if  $g(x, y + L) = g(x, y)$ , i.e. if  $g(x, y)$  is periodic in  $y$  with a period equal to  $L$  (the characteristic length of the reference periodicity cell  $Y$ ). Therefore we have that  $a_\varepsilon(x) = a\left(\frac{x}{\varepsilon}\right) = a(y)$  is  $Y$ -periodic function in  $y$ . We look for the solution of (2.7) in the form of the following two-scale asymptotic expansion:

$$u_\varepsilon(x) = u_0\left(x, \frac{x}{\varepsilon}\right) + \varepsilon u_1\left(x, \frac{x}{\varepsilon}\right) + \varepsilon^2 u_2\left(x, \frac{x}{\varepsilon}\right) \quad (2.9)$$

where all the terms  $u_0$ ,  $u_1$  and  $u_2$  are  $Y$ -periodic in  $y = \frac{x}{\varepsilon}$ . We want to investigate the behaviour of the PDE (2.7a) when  $\varepsilon \rightarrow 0$ . Now we plug the asymptotic expansion (2.9) in (2.7a) and taking into account that  $\nabla = \nabla_x + \frac{1}{\varepsilon} \nabla_y$ , we obtain

$$\begin{aligned} & - \left( \nabla_x + \frac{1}{\varepsilon} \nabla_y \right) \cdot \left( a(y) \left( \nabla_x + \frac{1}{\varepsilon} \nabla_y \right) \left( u_0(x, y) + \varepsilon u_1(x, y) + \varepsilon^2 u_2(x, y) \right) \right) = f(x) \iff \\ & - \left( \nabla_x + \frac{1}{\varepsilon} \nabla_y \right) \cdot \left( a(y) \left( \frac{1}{\varepsilon} \nabla_y u_0 + \nabla_x u_0 + \nabla_y u_1 + \varepsilon \nabla_x u_1 + \varepsilon \nabla_y u_2 + \varepsilon^2 \nabla_x u_2 \right) \right) = f(x) \end{aligned} \quad (2.10)$$

which is equivalent to

$$\begin{aligned}
& -\frac{1}{\varepsilon^2} \nabla_y \cdot (a(y) \nabla_y u_0) - \frac{1}{\varepsilon} \nabla_y \cdot (a(y) \nabla_x u_0 + a(y) \nabla_y u_1) - \\
& -\nabla_y \cdot (a(y) \nabla_x u_1 + a(y) \nabla_y u_2) - \varepsilon \nabla_y \cdot (a(y) \nabla_x u_2) - \frac{1}{\varepsilon} \nabla_x \cdot (a(y) \nabla_y u_0) - \\
& -\nabla_x \cdot (a(y) \nabla_x u_0 + a(y) \nabla_y u_1) - \varepsilon \nabla_x \cdot (a(y) \nabla_x u_1 + a(y) \nabla_y u_2) + O(\varepsilon^2) = f(x) \quad (2.11)
\end{aligned}$$

Finally we obtain

$$\begin{aligned}
& -\frac{1}{\varepsilon^2} \nabla_y \cdot (a(y) \nabla_y u_0) - \\
& -\frac{1}{\varepsilon} [\nabla_y \cdot (a(y) \nabla_x u_0 + a(y) \nabla_y u_1) + \nabla_x \cdot (a(y) \nabla_y u_0)] - \\
& -\varepsilon^0 [\nabla_y \cdot (a(y) \nabla_x u_1 + a(y) \nabla_y u_2) + \nabla_x \cdot (a(y) \nabla_x u_0 + a(y) \nabla_y u_1)] + \\
& +O(\varepsilon) = f(x) \quad (2.12)
\end{aligned}$$

Since the latter equality must be true for each  $x \in \Omega$ , we equal like powers of  $\varepsilon$ . This way we obtain the following equations for  $u_0(x, y)$  and the first and second order correctors  $u_1(x, y)$  and  $u_2(x, y)$  respectively:

$$\varepsilon^{-2} : -\nabla_y \cdot (a(y) \nabla_y u_0) = 0 \quad (2.13a)$$

$$\varepsilon^{-1} : -[\nabla_y \cdot (a(y) \nabla_x u_0 + a(y) \nabla_y u_1) + \nabla_x \cdot (a(y) \nabla_y u_0)] = 0 \quad (2.13b)$$

$$\varepsilon^0 : -[\nabla_y \cdot (a(y) \nabla_x u_1 + a(y) \nabla_y u_2) + \nabla_x \cdot (a(y) \nabla_x u_0 + a(y) \nabla_y u_1)] = f(x) \quad (2.13c)$$

### 2.1.1 Order $\varepsilon^{-2}$

We obtain the following equation for  $u_0(x, y)$ :

$$-\nabla_y \cdot (a(y) \nabla_y u_0) = 0, \quad (x, y) \in [\Omega \times Y] \quad (2.14)$$

and we will show that  $u_0$  is a function only of  $x$ .

We want to solve equation (2.14) with respect to the  $y$  variable, assuming that  $x$  is a given constant. Therefore we write the weak formulation of equation (2.14) and after applying the divergence theorem we obtain

$$\begin{aligned}
& -\int_Y \nabla_y \cdot (a(y) \nabla_y u_0) v(y) dy = 0, \quad \forall v(y) \in H_{per}^1(Y) \iff \\
& \int_Y \nabla_y \cdot (v(y) a(y) \nabla_y u_0) dy - \int_Y a(y) \nabla_y u_0 \cdot \nabla_y v dy = 0, \quad \forall v(y) \in H_{per}^1(Y) \iff \\
& \underbrace{\int_{\partial Y} v(y) a(y) \nabla_y u_0 \cdot \mathbf{n} ds}_{=0} - \int_Y a(y) \nabla_y u_0 \cdot \nabla_y v dy = 0, \quad \forall v(y) \in H_{per}^1(Y) \iff \\
& -\int_Y a(y) \nabla_y u_0 \cdot \nabla_y v dy = 0, \quad \forall v(y) \in H_{per}^1(Y) \quad (2.15)
\end{aligned}$$

In the latter equality we have that  $\int_{\partial Y} v(y)a(y)\nabla_y u_0 \cdot \mathbf{n} ds = 0$  due to symmetry ( we assume that the reference periodicity cell is symmetric, see Figure 2) and periodicity ( we have periodic microstructure, i.e. all the functions  $v(y)$ ,  $a(y)$  and  $u_0(x, y)$  are  $Y$ -periodic with respect to the  $y$  variable which means that these functions take equal values on the opposite sides of the periodicity cell  $Y$  and the unit normal vectors  $\mathbf{n}$  are collinear but pointing in opposite directions). Therefore for the weak formulation we obtain

$$\int_Y a(y)\nabla_y u_0 \cdot \nabla_y v dy = 0, \quad \forall v(y) \in H^1_{per}(Y) \quad (2.16)$$

Since (2.16) is true for each  $Y$ -periodic test function in  $H^1(Y)$ , we can take as test function  $v(y) = u_0(x, y)$  (assuming  $x$  is constant) and thus we obtain

$$\begin{aligned} \int_Y a(y)\nabla_y u_0 \cdot \nabla_y u_0 dy &= 0 \iff & (2.17) \\ 0 \leq \int_Y a(y) \sum_i \left( \frac{\partial u_0}{\partial y_i} \right)^2 dy &= 0 \quad (a(y) > 0, \forall y \in Y) \iff \\ & \left( \frac{\partial u_0}{\partial y_i} \right)^2 = 0, \quad \forall i \iff \\ & \frac{\partial u_0}{\partial y_i} = 0, \quad \forall i \iff \\ & u_0 = u_0(x) \end{aligned} \quad (2.18)$$

which means that  $u_0$  does not depend on the  $y$  variable.

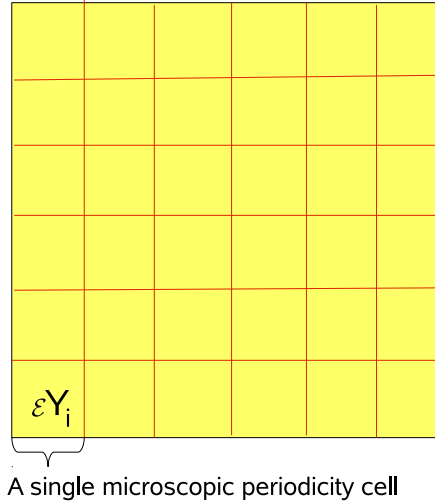


Figure 2: Periodic media

### 2.1.2 Order $\varepsilon^{-1}$

We have the following equation for the first order corrector  $u_1(x, y)$ :

$$- [\nabla_y \cdot (a(y)\nabla_x u_0 + a(y)\nabla_y u_1) + \nabla_x \cdot (a(y)\nabla_y u_0)] = 0 \quad (2.19)$$



where  $\nabla_y u_0(x) = 0$  and therefore the latter equation becomes

$$\nabla_y \cdot (a(y)\nabla_x u_0 + a(y)\nabla_y u_1) = 0 \quad (2.20)$$

which is equivalent to

$$\nabla_y \cdot (a(y)\nabla_y u_1) = -\nabla_y \cdot (a(y)\nabla_x u_0) \quad (2.21)$$

Now we seek the solution  $u_1$  in the following form

$$u_1(x, y) = \nabla_x u_0 \cdot \varphi \quad (2.22)$$

where  $\varphi(y) = (\varphi_1(y), \varphi_2(y))$  is a vector function. Thus

$$u_1(x, y) = \sum_{i=1}^2 \frac{\partial u_0}{\partial x_i}(x) \varphi_i(y) \quad (2.23)$$

And we obtain that  $u_1 = \nabla_x u_0 \cdot \varphi$  is a solution of (2.21) if and only if the  $Y$ -periodic functions  $\varphi_i(y)$  satisfy the following auxiliary cell problems

$$-\nabla_y \cdot (a(y)\nabla_y \varphi_i) = \frac{\partial a}{\partial y_i}, \quad i = 1, 2, y \in Y \quad (2.24)$$

### 2.1.3 Order $\varepsilon^0$

From (2.13c) we have

$$-\nabla_y \cdot (a(y)\nabla_x u_1 + a(y)\nabla_y u_2) - \nabla_x \cdot (a(y)\nabla_x u_0 + a(y)\nabla_y u_1) = f(x) \quad (2.25)$$

Now we integrate both sides of the equality over the periodicity cell  $Y$  and we divide by the measure of  $Y$

$$\begin{aligned} & -\frac{1}{|Y|} \int_Y \nabla_y \cdot (a(y)\nabla_x u_1 + a(y)\nabla_y u_2) \, dy - \\ & -\frac{1}{|Y|} \int_Y \nabla_x \cdot (a(y)\nabla_x u_0 + a(y)\nabla_y u_1) \, dy = f(x) \iff \\ & -\frac{1}{|Y|} \underbrace{\int_{\partial Y} (a(y)\nabla_x u_1 + a(y)\nabla_y u_2) \cdot \mathbf{n} \, ds}_{=0} - \\ & -\frac{1}{|Y|} \int_Y \nabla_x \cdot (a(y)\nabla_x u_0 + a(y)\nabla_y u_1) \, dy = f(x) \iff \\ & -\frac{1}{|Y|} \int_Y \nabla_x \cdot (a(y)\nabla_x u_0 + a(y)\nabla_y u_1) \, dy = f(x) \end{aligned} \quad (2.26)$$

We substitute  $u_1 = \sum_{i=1}^2 \frac{\partial u_0}{\partial x_i}(x) \varphi_i(y)$  and  $\nabla_x u_0 = \sum_{i=1}^2 \frac{\partial u_0}{\partial x_i} \vec{e}_i$ , and we obtain

$$\begin{aligned}
& -\frac{1}{|Y|} \int_Y \nabla_x \cdot \left( a(y) \nabla_x u_0 + a(y) \sum_{i=1}^2 \frac{\partial u_0}{\partial x_i}(x) \nabla_y \varphi_i \right) dy = f(x) \iff \\
& -\frac{1}{|Y|} \nabla_x \cdot \left( \int_Y \left( a(y) \nabla_x u_0 + a(y) \sum_{i=1}^2 \frac{\partial u_0}{\partial x_i}(x) \nabla_y \varphi_i \right) dy \right) = f(x) \iff \\
& -\frac{1}{|Y|} \nabla_x \cdot \left( \left( \int_Y a(y) dy \right) \nabla_x u_0 + \sum_{i=1}^2 \frac{\partial u_0}{\partial x_i}(x) \left( \int_Y a(y) \nabla_y \varphi_i dy \right) \right) = f(x) \iff \\
& -\frac{1}{|Y|} \nabla_x \cdot \left( \left( \int_Y a(y) dy \right) \sum_{i=1}^2 \frac{\partial u_0}{\partial x_i} \vec{e}_i + \sum_{i=1}^2 \frac{\partial u_0}{\partial x_i}(x) \left( \int_Y a(y) \nabla_y \varphi_i dy \right) \right) = f(x) \iff \\
& -\frac{1}{|Y|} \nabla_x \cdot \left( \sum_{i=1}^2 \frac{\partial u_0}{\partial x_i} \left( \int_Y a(y) dy \right) \vec{e}_i + \sum_{i=1}^2 \frac{\partial u_0}{\partial x_i} \left( \int_Y a(y) \nabla_y \varphi_i dy \right) \right) = f(x) \iff \\
& -\frac{1}{|Y|} \nabla_x \cdot \left( \sum_{i=1}^2 \frac{\partial u_0}{\partial x_i} \left( \int_Y a(y) \vec{e}_i dy + \int_Y a(y) \nabla_y \varphi_i dy \right) \right) = f(x) \iff \\
& -\nabla_x \cdot \left( \sum_{i=1}^2 \frac{\partial u_0}{\partial x_i} \left( \frac{1}{|Y|} \int_Y a(y) (\vec{e}_i + \nabla_y \varphi_i) dy \right) \right) = f(x) \tag{2.27}
\end{aligned}$$

where

$$\vec{e}_1 + \nabla_y \varphi_1 = \left( 1 + \frac{\partial \varphi_1}{\partial y_1}, \frac{\partial \varphi_1}{\partial y_2} \right) \tag{2.28}$$

$$\vec{e}_2 + \nabla_y \varphi_2 = \left( \frac{\partial \varphi_2}{\partial y_1}, 1 + \frac{\partial \varphi_2}{\partial y_2} \right) \tag{2.29}$$

$$\begin{aligned}
& \sum_{i=1}^2 \frac{\partial u_0}{\partial x_i} \left( \frac{1}{|Y|} \int_Y a(y) (\vec{e}_i + \nabla_y \varphi_i) dy \right) = \\
& = \begin{pmatrix} \frac{1}{|Y|} \int_Y a(y) \left( 1 + \frac{\partial \varphi_1}{\partial y_1} \right) dy & \frac{1}{|Y|} \int_Y a(y) \frac{\partial \varphi_2}{\partial y_1} dy \\ \frac{1}{|Y|} \int_Y a(y) \frac{\partial \varphi_1}{\partial y_2} dy & \frac{1}{|Y|} \int_Y a(y) \left( 1 + \frac{\partial \varphi_2}{\partial y_2} \right) dy \end{pmatrix} \begin{pmatrix} \frac{\partial u_0}{\partial x_1} \\ \frac{\partial u_0}{\partial x_2} \end{pmatrix} \tag{2.30}
\end{aligned}$$

Thus we obtain the homogenized problem

$$-\nabla_x \cdot (a_H \nabla_x u_0) = f(x), \quad x \in \Omega, \tag{2.31a}$$

$$u_0(x) = 0, \quad x \in \partial\Omega \tag{2.31b}$$

where the homogenized coefficient  $a_H$  (constant) is the following tensor

$$(a_H)_{i,j=1}^2 = \frac{1}{|Y|} \int_Y a(y) \left( \delta_{ij} + \frac{\partial \varphi_j}{\partial y_i}(y) \right) dy \tag{2.32}$$

### 2.1.4 Numerical Experiment

- $\Omega = [0, 1] \times [0, 1]$
- $Y = [0, 1] \times [0, 1]$
- We take  $a(x) = \cos(32\pi x_1) \cos(32\pi x_2) + 1.1 > 0$  and  $f(x) = 16$
- $\varepsilon = \frac{1}{16}$

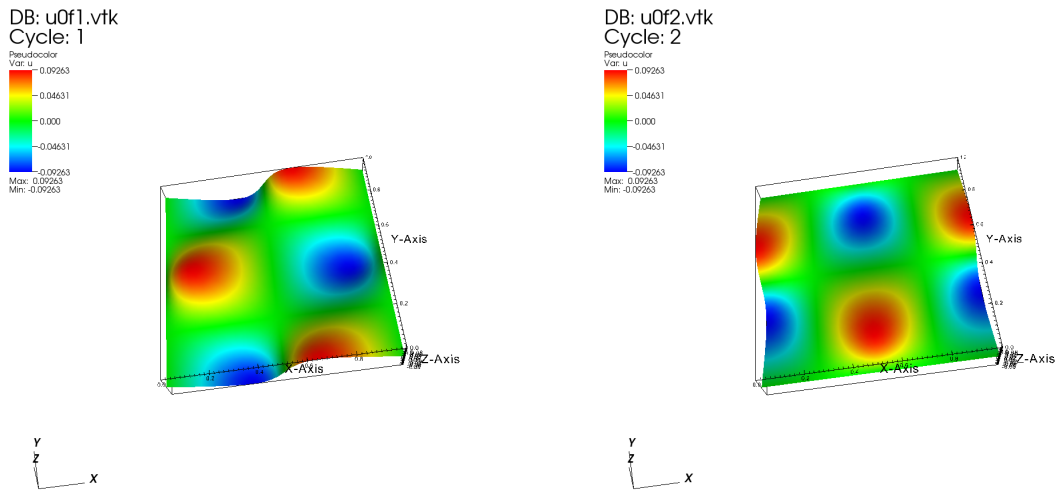
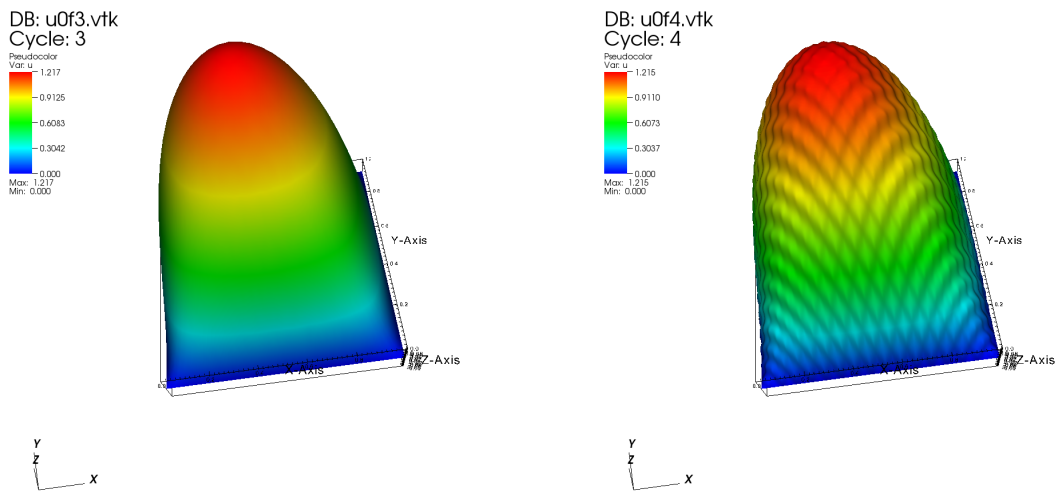


Figure 3: Solutions of the Cell Problems



(a) Homogenized Solution

(b) Exact Solution

Figure 4: Homogenized Solution and Exact Solution

### 3 Some Test Problems

#### 3.1 Nonlinear Elliptic Problem: Straightforward Approach

We consider the following nonlinear equation with periodic coefficient:

$$-\nabla \cdot (a_\varepsilon(x, u_\varepsilon) \nabla u_\varepsilon) = f(x), \quad x \in \Omega = [0, 1] \times [0, 1] \quad (3.1a)$$

$$u_\varepsilon(x) = 0, \quad x \in \partial\Omega \quad (3.1b)$$

where

- $a_\varepsilon(x, u_\varepsilon) > 0, \forall x \in \Omega$  (ellipticity condition), and we assume that  $a_\varepsilon(x, u_\varepsilon)$  is a smooth function  $\forall x \in \Omega$
- $\varepsilon = l/L$
- $L$  - characteristic length of the macrodomain  $\Omega$
- $l$  - characteristic length of the periodic microscale structures
- $a_\varepsilon(x, u_\varepsilon(x)) = a\left(\frac{x}{\varepsilon}, u_\varepsilon\right)$  is an oscillating coefficient with period  $\varepsilon L$
- We assume the following asymptotic expansion for the function  $u_\varepsilon$ :  

$$u_\varepsilon(x) = u_0(x) + \varepsilon u_1\left(x, \frac{x}{\varepsilon}\right) + \varepsilon^2 u_2\left(x, \frac{x}{\varepsilon}\right), \quad y = \frac{x}{\varepsilon}$$
- $a(y, u_\varepsilon) = a(y, u_0) + O(\varepsilon)$  for smooth functions  $a(y, u_\varepsilon)$  (Taylor series)
- We also have that the functions  $a(y, u_\varepsilon)$ ,  $u_1(x, y)$  and  $u_2(x, y)$  are  $Y$ -periodic in the  $y$  variable

##### 3.1.1 Homogenization: Order $\varepsilon^{-1}$

After we plug the asymptotic expansion of  $u_\varepsilon$  in (3.1a) and we identify equal powers of  $\varepsilon$ , for order  $\varepsilon^{-1}$  we obtain the following equation

$$\nabla_y \cdot (a(y, u_0) \nabla_y u_1) = -\nabla_y \cdot (a(y, u_0) \nabla_x u_0) \quad (3.2)$$

From (3.2) where we obtain that

$$u_1(x, y) = \sum_{l=1}^2 \chi_l(y) \frac{\partial u_0}{\partial x_l}(x) \quad (3.3)$$

where the  $Y$ -periodic functions  $\chi_l(y)$  are the solution of the following auxiliary cell problems:

$$\nabla \cdot (a(y, u_0(x)) \nabla_y \chi_l) = -\frac{\partial a}{\partial y_l}(y, u_0(x)), \quad y \in Y, \quad l = 1, 2 \quad (3.4)$$

Therefore we have to solve the cell problems for each integration point  $x \in \Omega$ .

We apply periodic boundary conditions on  $\partial Y$  (see Figure 5)

$$\begin{aligned} \nabla_y \chi_l \cdot \mathbf{n}|_{AD} &= \nabla_y \chi_l \cdot \mathbf{n}|_{BC} \\ \nabla_y \chi_l \cdot \mathbf{n}|_{AB} &= \nabla_y \chi_l \cdot \mathbf{n}|_{CD} \end{aligned}$$

and in order to fix the solution we impose

$$\int_Y \chi_l(y) dy = 0$$

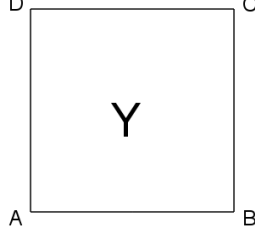


Figure 5: Solution Domain of the Auxiliary Cell Problems

### 3.1.2 Homogenization: Order $\varepsilon^0$

From the order  $\varepsilon^0$  equation we obtain the homogenized problem

$$-\nabla \cdot (a^*(u_0) \nabla u_0) = f(x), \quad x \in \Omega \quad (3.5a)$$

$$u_0(x) = 0, \quad x \in \partial\Omega \quad (3.5b)$$

where  $a^*(u_0)$  is the following tensor:

$$a^* = (a^*)_{i,j=1}^2 = \frac{1}{|Y|} \int_Y a(y, u_0) \left( \delta_{ij} + \frac{\partial \chi_j}{\partial y_i}(y) \right) dy \quad (3.6)$$

### 3.1.3 Numerical Experiment

We solve the following test problem:

- $-\nabla \cdot (a_\varepsilon(x, u_\varepsilon) \nabla u_\varepsilon) = f(x), \quad x \in \Omega = [0, 1] \times [0, 1]$
- $u_\varepsilon(x) = 0, \quad x \in \partial\Omega$
- $a_\varepsilon(x, u_\varepsilon) = k_\varepsilon(x) u_\varepsilon^2 + 1 > 0$ - ellipticity condition, where
- $k_\varepsilon(x) = \cos(32\pi x_1) \cos(32\pi x_2) + 1.1$
- $f(x) = 5$
- We have  $L = 32\pi$  and  $l = 2\pi$ , and therefore  $\varepsilon = \frac{1}{16} = 0.0625$ , and we have 256 periodicity cells
- Since the auxiliary cell problem depends on the macrosolution  $u_0(x)$ , we have to solve the cell problem for each integration point  $x$  in the macrodomain and at each Newton iteration

**Note:** From now on in all the numerical experiments we will refer to the numerical solution of the full microscale model as to the "exact solution".

	Nodes	Periodicity Cells	Time	Max	Min
Homogenized Problem	289	256	681s	1.163	1
Cell Problem	2113				
Exact Solution	65536	256	74s	1.173	1

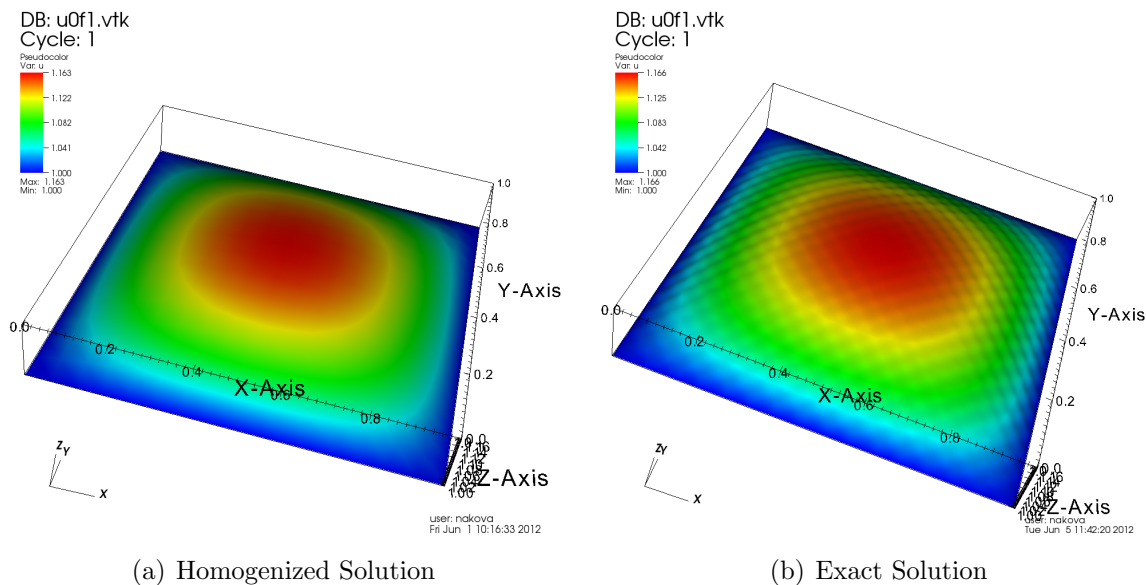


Figure 6: 289 Nodes for the Homogenized Problem and 2113 Nodes for the Cell Problems

	Nodes	Periodicity Cells	Time	Max	Min
Homogenized Problem	289	256	125s	1.163	1
Cell Problem	545				
Exact Solution	65536	256	74s	1.173	1

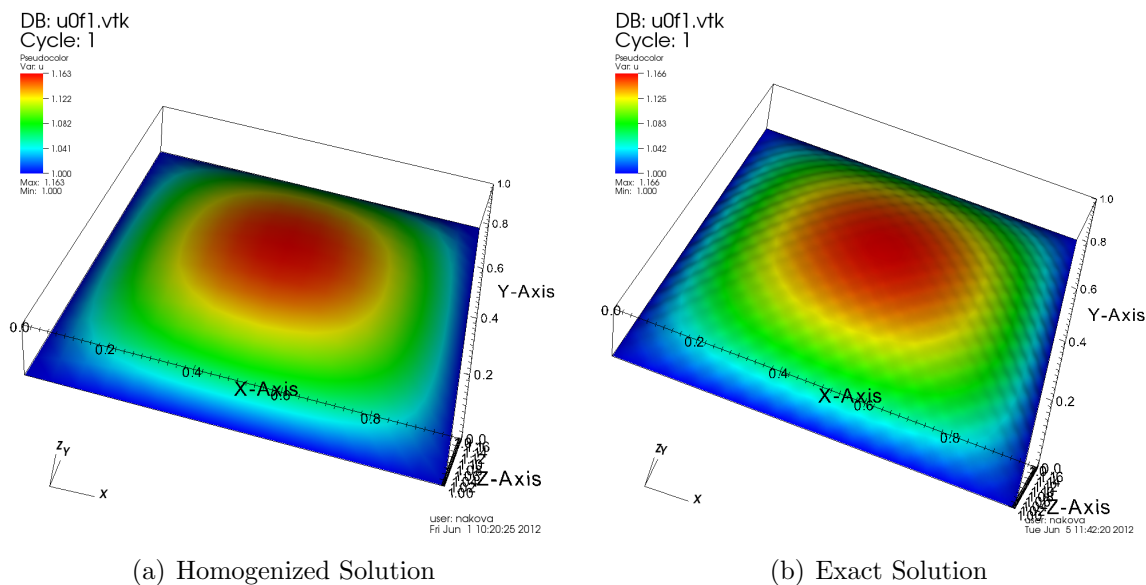


Figure 7: 289 Nodes for the Homogenized Problem and 545 Nodes for the Cell Problems

	Nodes	Periodicity Cells	Time	Max	Min
Homogenized Problem	289	256	36s	1.163	1
Cell Problem	145				
Exact Solution	65536	256	74s	1.173	1

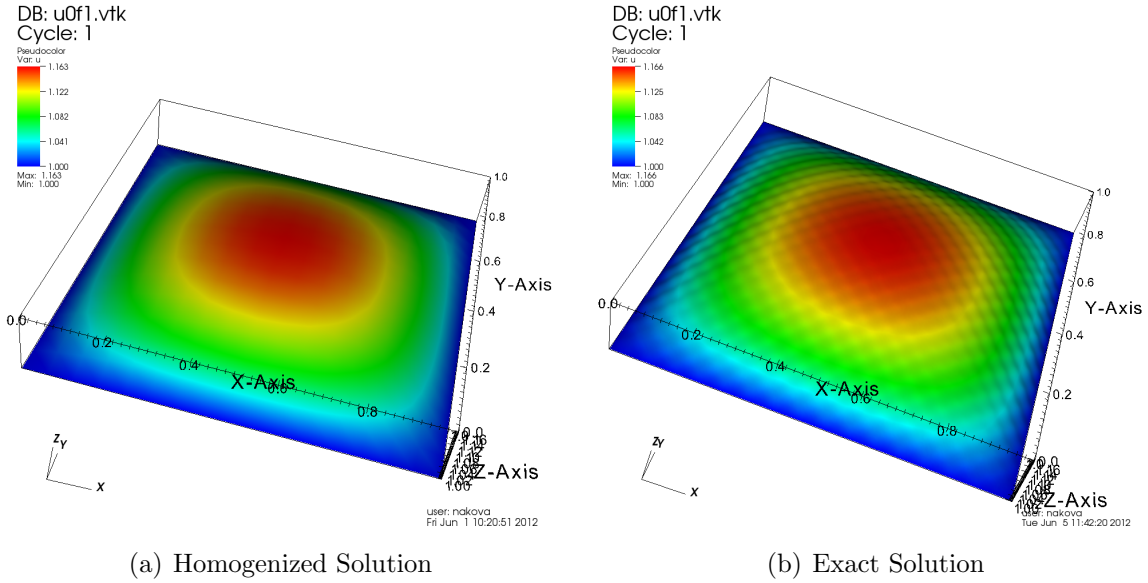


Figure 8: 289 Nodes for the Homogenized Problem and 145 Nodes for the Cell Problems

	Nodes	Periodicity Cells	Time	Max	Min
Homogenized Problem	81	256	31s	1.155	1
Cell Problem	545				
Exact Solution	65536	256	74s	1.173	1

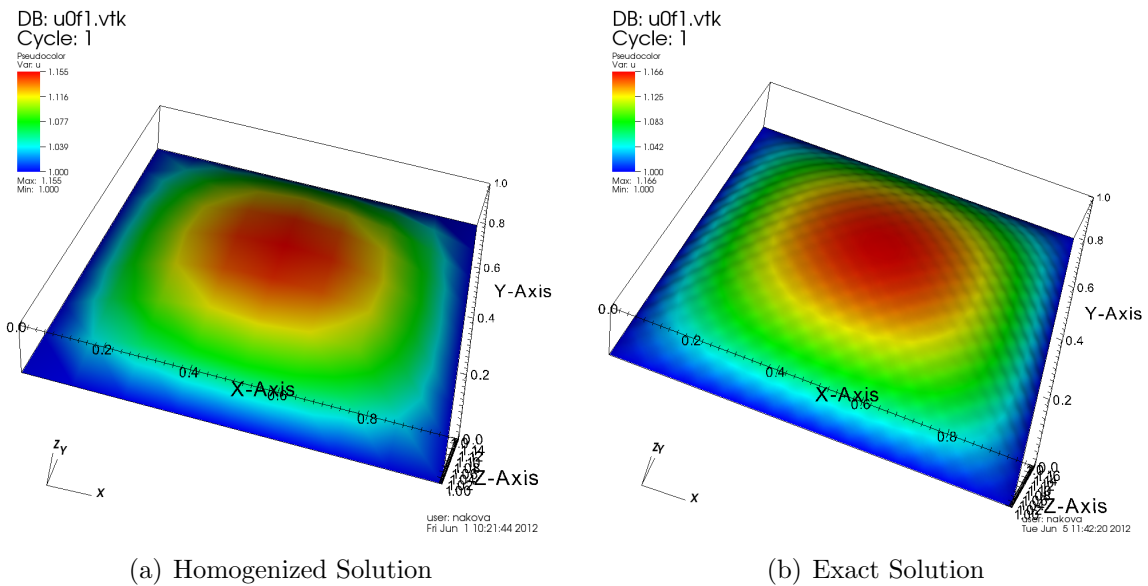


Figure 9: 81 Nodes for the Homogenized Problem and 545 Nodes for the Cell Problems

As we can see from the numerical results above, the computational time needed for solving the homogenized problem is larger than that needed for the full microscale

simulation. This is due to the fact that the considered problem is nonlinear and we have to solve a cell problem for each integration point  $x \in \Omega$ . In the case of nonlinear problems different optimizations and simplifications can be done in order to reduce the computational time. We will not discuss here this topic.

## 3.2 Nonlinear Elliptic Problem: Case Specific Optimization

We solve the following problem:

$$-\nabla \cdot (a_\varepsilon(x, u_\varepsilon(x)) \nabla u_\varepsilon) = f(x), \quad x \in \Omega = [0, 1] \times [0, 1] \quad (3.7a)$$

$$u_\varepsilon(x) = 1, \quad x \in \partial\Omega \quad (3.7b)$$

### 3.2.1 Cell Problem

The  $Y$ -periodic function  $\chi_l(y)$  is the solution of the following auxiliary cell problem:

$$\nabla_y \cdot (a(y, u_0) \nabla_y \chi_l) = -\frac{\partial a(y, u_0)}{\partial y_l}, \quad l = 1, 2 \quad (3.8)$$

which is equivalent to

$$\begin{aligned} \nabla_y \cdot (k(y) u_0^2(x) \nabla_y \chi_l) &= -\frac{\partial}{\partial y_l} (k(y) u_0^2(x)), \quad l = 1, 2 \iff \\ u_0^2(x) \nabla_y \cdot (k(y) \nabla_y \chi_l) &= -u_0^2(x) \frac{\partial k}{\partial y_l}(y), \quad l = 1, 2 \end{aligned} \quad (3.9)$$

Thus for the cell problem we obtain (since  $u_0(x) \neq 0$ )

$$\nabla_y \cdot (k(y) \nabla_y \chi_l) = -\frac{\partial k}{\partial y_l}(y), \quad l = 1, 2 \quad (3.10)$$

This means that we do not have to solve the cell problems for each point  $x \in \Omega$  of the macrodomain, but only once. Thus, due to the specific form of the coefficient  $a_\varepsilon(x, u_\varepsilon)$  we are able to entirely decouple the macro and the micro scales and to reduce significantly the computational time.

### 3.2.2 Homogenized Problem

We obtain the following homogenized problem:

$$-\nabla \cdot (a^*(u_0) \nabla u_0) = f(x), \quad x \in \Omega \quad (3.11a)$$

$$u_0(x) = 1, \quad x \in \partial\Omega \quad (3.11b)$$



where the homogenized coefficient  $a^*$  is given by

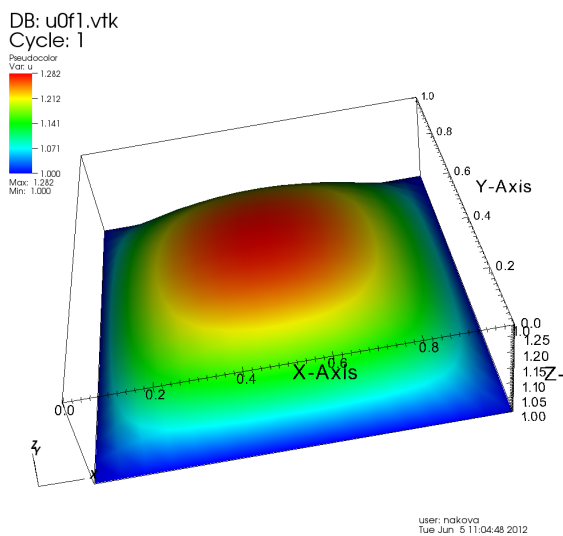
$$\begin{aligned}
 a^* &= (a^*)_{i,j=1}^2 = \frac{1}{|Y|} \int_Y a(y, u_0) \left( \delta_{ij} + \frac{\partial \chi_j}{\partial y_i}(y) \right) dy = \\
 &= \frac{1}{|Y|} \int_Y k(y) u_0^2 \left( \delta_{ij} + \frac{\partial \chi_j}{\partial y_i}(y) \right) dy = \\
 &= u_0^2(x) \underbrace{\frac{1}{|Y|} \int_Y k(y) \left( \delta_{ij} + \frac{\partial \chi_j}{\partial y_i}(y) \right) dy}_{\text{we calculate this integral only once}}
 \end{aligned} \tag{3.12}$$

### 3.2.3 Numerical Experiment

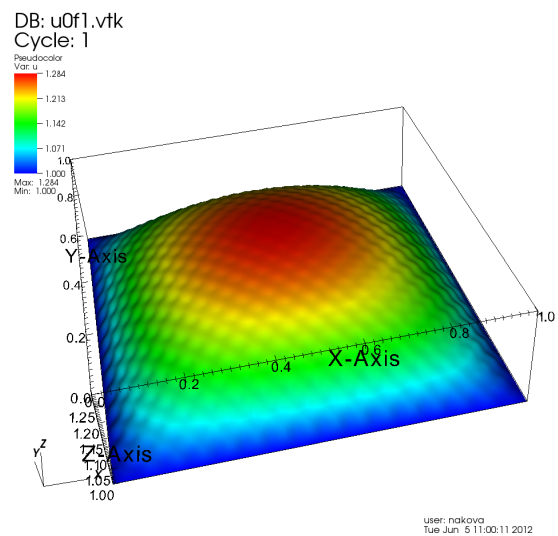
We have the following setting for our test problem:

- $\Omega = [0, 1] \times [0, 1]$
- $a_\varepsilon(x, u_\varepsilon) = k_\varepsilon(x) u_\varepsilon^2$
- $k_\varepsilon(x) = \cos(32\pi x_1) \cos(32\pi x_2) + 1.1$
- $f(x) = 5$
- $\varepsilon = 0.0625$

	Nodes	Periodicity Cells	Time	Max	Min
Homogenized Problem	289	256	0.27s	1.282	1
Cell Problem	145				
Exact Solution	16384	256	22s	1.284	1

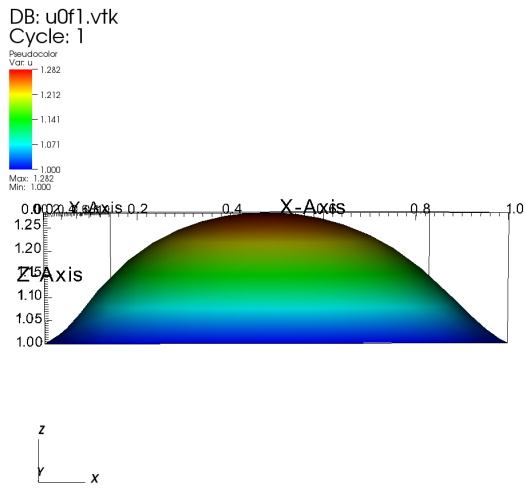


(a) Homogenized Solution

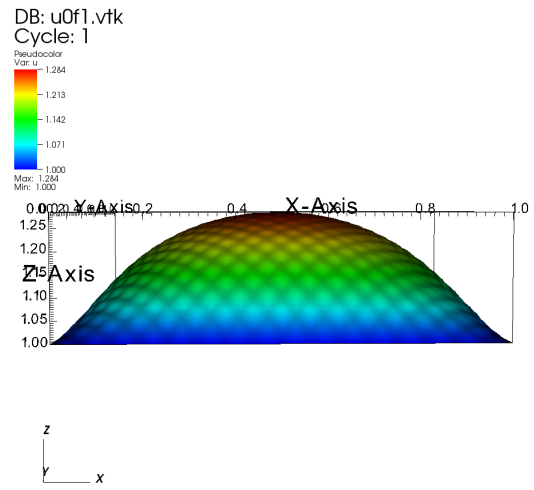


(b) Exact Solution

Figure 10: 289 Nodes for Solving the Homogenized Problem and 145 Nodes for the Cell Problems



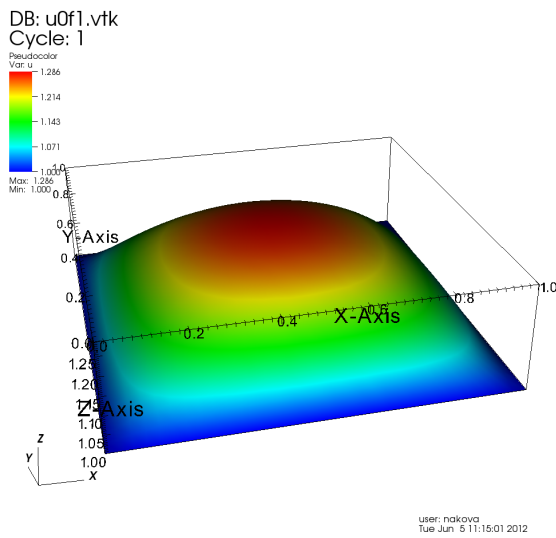
(a) Homogenized Solution



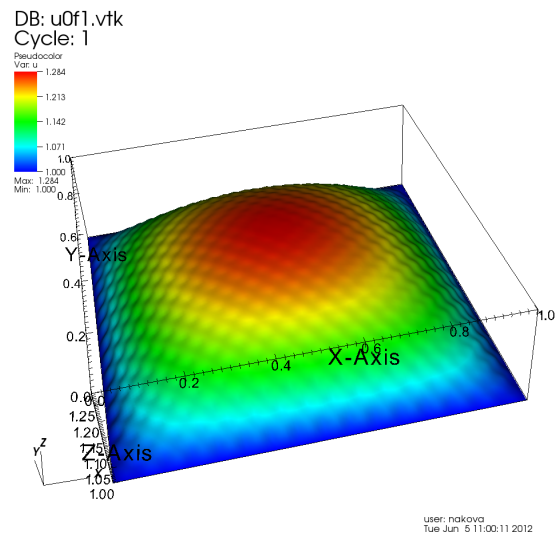
(b) Exact Solution

Figure 11: 289 Nodes for Solving the Homogenized Problem and 145 Nodes for the Cell Problems: Side View

	Nodes	Periodicity Cells	Time	Max	Min
Homogenized Problem	1089	256	0.98s	1.286	1
Cell Problem	145				
Exact Solution	16384	256	22s	1.284	1

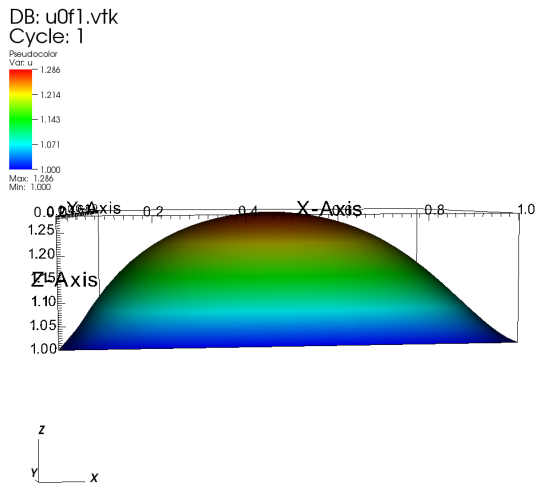


(a) Homogenized Solution

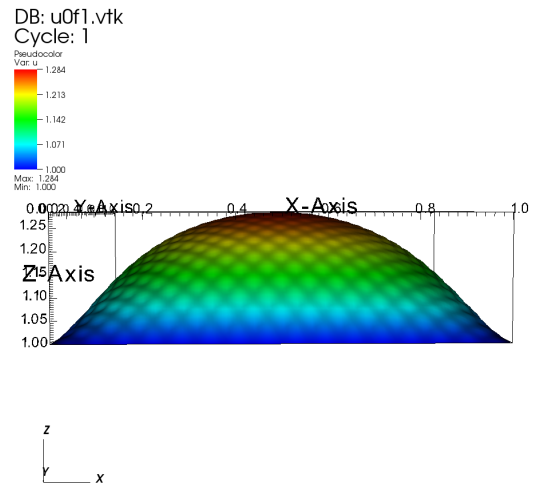


(b) Exact Solution

Figure 12: 1089 Nodes for Solving the Homogenized Problem and 145 Nodes for the Cell Problems



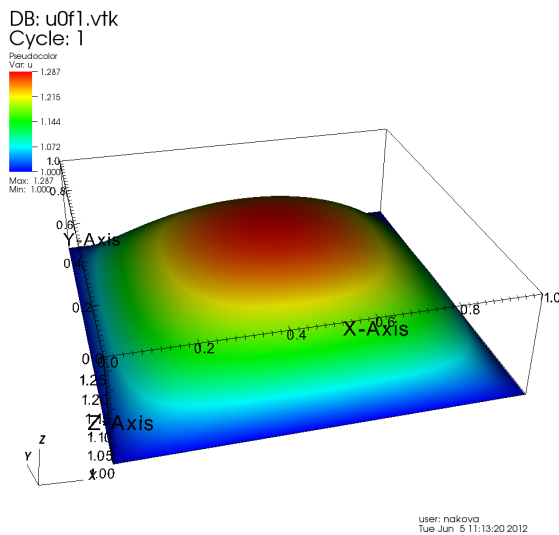
(a) Homogenized Solution



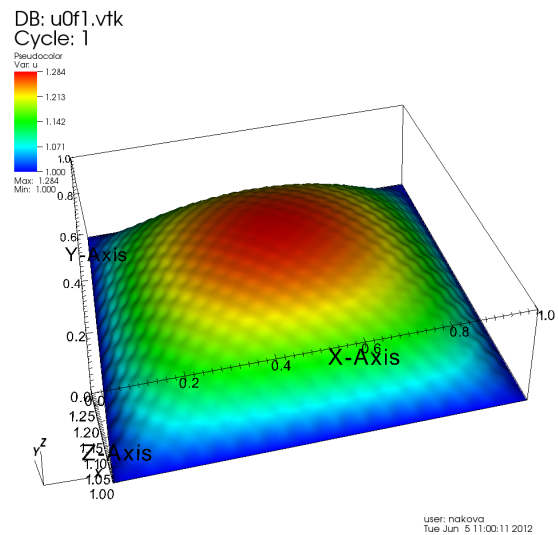
(b) Exact Solution

Figure 13: 1089 Nodes for Solving the Homogenized Problem and 145 Nodes for the Cell Problems: Side View

	Nodes	Periodicity Cells	Time	Max	Min
Homogenized Problem	1089	256	1.05s	1.287	1
Cell Problem	545				
Exact Solution	16384	256	22s	1.284	1



(a) Homogenized Solution



(b) Exact Solution

Figure 14: 1089 Nodes for Solving the Homogenized Problem and 545 Nodes for the Cell Problems

## 4 Lithium-ion Batteries: Mathematical Model

We consider the microscale mathematical model derived in [8].

We use the following notation:

- $\Omega$  - domain of the whole battery cell
- $\partial\Omega$  - boundary of  $\Omega$
- $\Omega_e$  - domain of the electrolyte
- $\Omega_a$  - domain of the anode active particles
- $\partial\Omega_a$  - boundary of  $\Omega_a$
- $\Omega_c$  - domain of the cathode active particles
- $\partial\Omega_c$  - boundary of  $\Omega_c$
- $\Omega_s = \Omega_a \cup \Omega_c$  - domain of the solid active particles

### 4.1 Equations of the Electrolyte

The equations of the electrolyte phase couple the concentration  $c^e$  of lithium ions and the potential  $\phi^e$  in the electrolyte and they have the following form

$$\frac{\partial c^e}{\partial t} - \nabla \cdot (k_{11}^e(c^e)\nabla c^e + k_{12}^e\nabla\phi^e) = 0, \quad x \in \Omega_e \quad (4.1a)$$

$$-\nabla \cdot (k_{21}^e(c^e)\nabla c^e + k_{22}^e\nabla\phi^e) = 0, \quad x \in \Omega_e \quad (4.1b)$$

where for the coefficients we have

$$k_{11}^e(c^e) = D^e + \frac{RT}{F^2} \frac{(t_+)^2 \kappa^e}{c^e} \quad (4.2a)$$

$$k_{12}^e = \kappa^e \frac{t_+}{F} \quad (4.2b)$$

$$k_{21}^e(c^e) = \frac{RT}{F} \frac{\kappa^e t_+}{c^e} \quad (4.2c)$$

$$k_{22}^e = \kappa^e \quad (4.2d)$$

with

- $c^e$  - concentration of Li+ in the electrolyte
- $\phi^e$  - potential in the electrolyte
- $\kappa^e$ -ion conductivity
- $D^e$ -interdiffusion coefficient

## 4.2 Equations of the Solid

The equations describing the transport of Lithium ions and charge in the solid active particles are

$$\frac{\partial c^s}{\partial t} - \nabla \cdot (D^s \nabla c^s) = 0, \quad x \in \Omega_s \quad (4.3a)$$

$$-\nabla \cdot (\kappa^s \nabla \phi^s) = 0, \quad x \in \Omega_s \quad (4.3b)$$

where

- $c^s$  - concentration of Li+ in the active particles
- $\phi^s$  - potential in the active particles
- $D^s$ -ion diffusion
- $\kappa^s$ -electronic conductivity

We make no distinction between anode and cathode active particles since the equations describing the electrochemical processes in both type of particles are identical. We only have different values for the diffusion coefficient  $D^s$  and the electronic conductivity  $\kappa^s$ .

## 4.3 Interface Conditions

The ion flux and the electrical current in the electrolyte are respectively:

$$\mathbf{N}^e = - (k_{11}^e (c^e) \nabla c^e + k_{12}^e \nabla \phi^e) \quad (4.4a)$$

$$\mathbf{J}^e = - (k_{21}^e (c^e) \nabla c^e + k_{22}^e \nabla \phi^e) \quad (4.4b)$$

The ion flux and the electrical current in the active particles are respectively:

$$\mathbf{N}^s = -D^s \nabla c^s \quad (4.5a)$$

$$\mathbf{J}^s = -\kappa^s \nabla \phi^s \quad (4.5b)$$

We have the following interface conditions, which are imposed on the boundary between the active particles and the electrolyte:

$$\mathbf{N}^s \cdot \mathbf{n}_s = \mathbf{N}^e \cdot \mathbf{n}_s = \mathcal{N}(c^e, c^s, \phi^e, \phi^s), \quad x \in \gamma \quad (4.6)$$

$$\mathbf{J}^s \cdot \mathbf{n}_s = \mathbf{J}^e \cdot \mathbf{n}_s = \mathcal{J}(c^e, c^s, \phi^e, \phi^s), \quad x \in \gamma \quad (4.7)$$

The unit normal vector  $\mathbf{n}_s$  points in the direction from the solid particles to the electrolyte. where  $\gamma$  is the interface boundary between the solid and the electrolyte and the current densities  $\mathcal{N}$  and  $\mathcal{J}$  are given by:

$$\mathcal{N} = \frac{k}{F} \sqrt{c^e c^s (c_{max}^s - c^s)} \left[ \exp \frac{F\eta}{2RT} - \exp \frac{-F\eta}{2RT} \right] \quad (4.8)$$

$$\mathcal{J} = F\mathcal{N} \quad (4.9)$$

- $\eta = \phi^s - \phi^e - U_0(c^s)$ , where  $U_0(c^s)$  is the open circuit potential

## 4.4 Boundary Conditions

With  $\omega_1$  and  $\omega_2$  we denote the outer anode and cathode boundary walls as shown in Figure 15. On the anode particles boundary  $\omega_1 \cap \partial\Omega_a$  we impose constant potential  $\phi^s$  and on the cathode particles boundary  $\omega_2 \cap \partial\Omega_c$  - constant applied current.

- Dirichlet boundary conditions:  $\phi^s(x) = E_1^s = const, \quad x \in \omega_1 \cap \partial\Omega_a$
- Neumann boundary conditions:

$$(\kappa^s \nabla \phi^s) \cdot \mathbf{n} = E_2^s = const, \quad x \in \omega_2 \cap \partial\Omega_c \quad (4.10)$$

$$\nabla c^s \cdot \mathbf{n} = 0, \quad x \in \{\omega_1 \cap \partial\Omega_a\} \cup \{\omega_2 \cap \partial\Omega_c\} \quad (4.11)$$

$$\mathbf{N}^e \cdot \mathbf{n} = \mathbf{J}^e \cdot \mathbf{n} = 0, \quad x \in \partial\Omega \quad (4.12)$$

$$\mathbf{N}^s \cdot \mathbf{n} = \mathbf{J}^s \cdot \mathbf{n} = 0, \quad x \in \partial\Omega \setminus \{\omega_1 \cup \omega_2\} \quad (4.13)$$

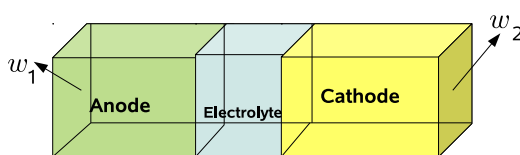


Figure 15: Battery Cell

## 5 Homogenization of the Li-ion Battery Model

We consider periodic arrangement of the active particles as shown in Figure 16 ([11]). As a single periodic cell we consider a cubic block consisting of one active particle surrounded by electrolyte as shown in Figure 17.

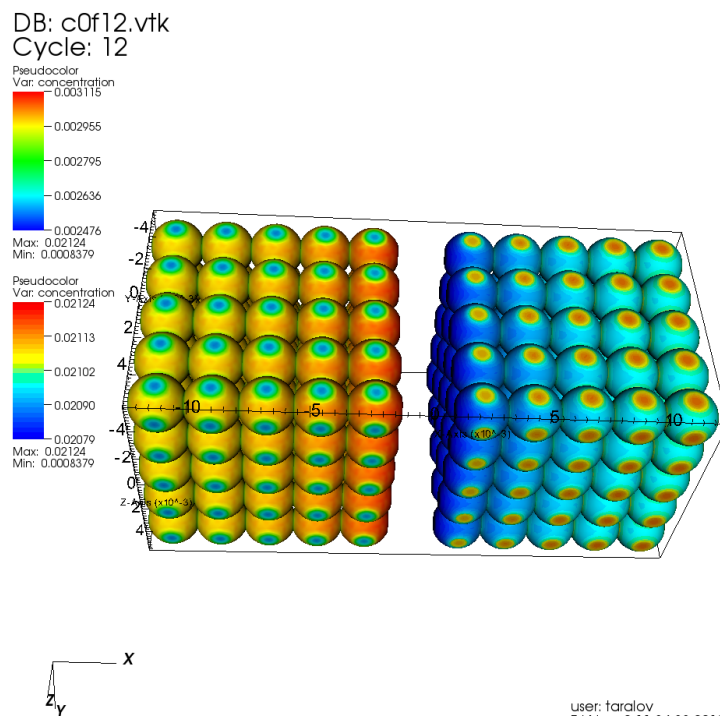


Figure 16: Battery Cell

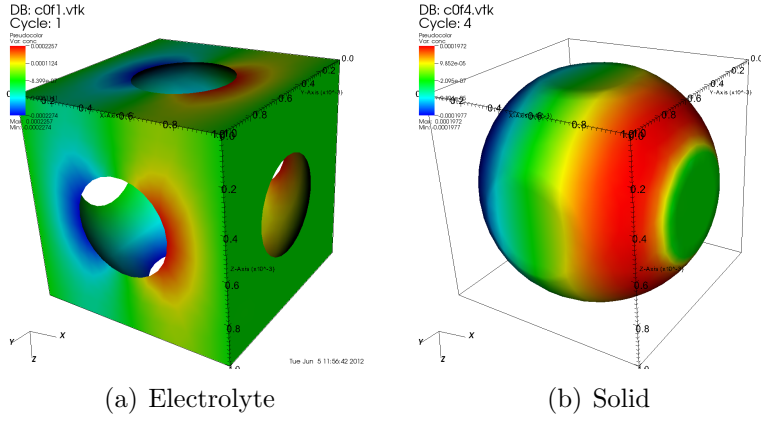


Figure 17: Geometry of the Periodicity Cell

We start by defining the model equations in the whole domain  $\Omega = \Omega_s \cup \Omega_e$ ,  $\Omega \in \mathbb{R}^3$

$$\frac{\partial(\chi^e(x)c^e)}{\partial t} - \nabla \cdot (k_{11}(x, c^e)\nabla c^e + k_{12}(x)\nabla\phi^e) = 0, \quad x \in \Omega \quad (5.1a)$$

$$-\nabla \cdot (k_{21}(x, c^e)\nabla c^e + k_{22}(x)\nabla\phi^e) = 0, \quad x \in \Omega \quad (5.1b)$$

$$\frac{\partial(\chi^s(x)c^s)}{\partial t} - \nabla \cdot (D(x)\nabla c^s) = 0, \quad x \in \Omega \quad (5.1c)$$

$$-\nabla \cdot (\kappa(x)\nabla\phi^s) = 0, \quad x \in \Omega \quad (5.1d)$$

with the boundary conditions:

- Dirichlet BC:  $\phi^s(x) = E_1^s = \text{const}$ ,  $x \in \omega_1$
- Neumann BC:

$$(\kappa(x)\nabla\phi^s) \cdot \mathbf{n} = E_2(x) = \chi^s(x)E_2^s, \quad x \in \omega_2 \quad (5.2)$$

$$\nabla c^s \cdot \mathbf{n} = 0, \quad x \in \omega_1 \cup \omega_2 \quad (5.3)$$

$$\mathbf{N}^e \cdot \mathbf{n} = \mathbf{J}^e \cdot \mathbf{n} = 0, \quad x \in \partial\Omega \quad (5.4)$$

where

$$k_{11}(x, c^e) = \chi^e(x)k_{11}^e(c^e) = \begin{cases} k_{11}^e(c^e), & x \in \Omega_e \\ 0, & x \in \Omega_s \end{cases}$$

$$k_{12}(x) = \chi^e(x)k_{12}^e = \begin{cases} k_{12}^e, & x \in \Omega_e \\ 0, & x \in \Omega_s \end{cases}$$

$$k_{21}(x, c^e) = \chi^e(x)k_{21}^e(c^e) = \begin{cases} k_{21}^e(c^e), & x \in \Omega_e \\ 0, & x \in \Omega_s \end{cases}$$

$$k_{22}(x) = \chi^e(x)k_{22}^e = \begin{cases} k_{22}^e, & x \in \Omega_e \\ 0, & x \in \Omega_s \end{cases}$$

$$D(x) = \chi^s(x)D^s = \begin{cases} 0, & x \in \Omega_e \\ D^s, & x \in \Omega_s \end{cases}$$

$$\kappa(x) = \chi^s(x)\kappa^s = \begin{cases} 0, & x \in \Omega_e \\ \kappa^s, & x \in \Omega_s \end{cases}$$

and

$$\chi^e(x) = \begin{cases} 1, & x \in \Omega_e \\ 0, & x \in \Omega_s \end{cases}$$

$$\chi^s(x) = \begin{cases} 0, & x \in \Omega_e \\ 1, & x \in \Omega_s \end{cases}$$

## 5.1 Asymptotic Analysis

We use the following notation

- $L$  - characteristic length of the electrodes
- $l$  - characteristic length of the active particles which in our case we consider to be the diameter of the "spherical-like" particle shown on Figure 17
- $\varepsilon = \frac{l}{L} \rightarrow 0$ ,  $y = \frac{x}{\varepsilon}$ , periodic structure with a reference periodicity cell  $Y = E \cup S$ , where
- $Y \sim L$ , i.e. the characteristic length of the reference periodicity cell is  $L$
- $E$  - electrolyte domain in the reference periodicity cell
- $S$  - solid particle domain in the reference periodicity cell
- $\Gamma$  - interface between the electrolyte and the particle in the reference periodicity cell

Now we write the problem in terms of a dependence on the small parameter  $\varepsilon$  and then we want to investigate the behaviour of the partial differential equations when  $\varepsilon$  goes to zero.

$$\frac{\partial (\chi_\varepsilon^e(x)c_\varepsilon^e)}{\partial t} - \nabla \cdot ((k_{11})_\varepsilon(x, c_\varepsilon^e)\nabla c_\varepsilon^e + (k_{12})_\varepsilon(x)\nabla \phi_\varepsilon^e) = 0, \quad x \in \Omega \quad (5.5a)$$

$$-\nabla \cdot ((k_{21})_\varepsilon(x, c_\varepsilon^e)\nabla c_\varepsilon^e + (k_{22})_\varepsilon(x)\nabla \phi_\varepsilon^e) = 0, \quad x \in \Omega \quad (5.5b)$$

$$\frac{\partial (\chi_\varepsilon^s(x)c_\varepsilon^s)}{\partial t} - \nabla \cdot (D_\varepsilon(x)\nabla c_\varepsilon^s) = 0, \quad x \in \Omega \quad (5.5c)$$

$$-\nabla \cdot (\kappa_\varepsilon(x)\nabla \phi_\varepsilon^s) = 0, \quad x \in \Omega \quad (5.5d)$$

with the following boundary conditions

- Dirichlet BC:  $\phi_\varepsilon^s(x) = E_1^s = const$ ,  $x \in \omega_1$
- Neumann BC:

$$(\kappa_\varepsilon(x)\nabla \phi_\varepsilon^s) \cdot \mathbf{n} = E_2^\varepsilon(x) = \chi_\varepsilon^s(x)E_2^s = \chi^s\left(\frac{x}{\varepsilon}\right)E_2^s, \quad x \in \omega_2 \quad (5.6)$$

$$\nabla c_\varepsilon^s \cdot \mathbf{n} = 0, \quad x \in \omega_1 \cup \omega_2 \quad (5.7)$$

$$\mathbf{N}_\varepsilon^e \cdot \mathbf{n} = \mathbf{J}_\varepsilon^e \cdot \mathbf{n} = 0, \quad x \in \partial\Omega \quad (5.8)$$

and interface conditions

$$-((k_{11})_\varepsilon\nabla c_\varepsilon^e + (k_{12})_\varepsilon\nabla \phi_\varepsilon^e) \cdot \mathbf{n}_s = \mathcal{N}_\varepsilon, \quad x \in \gamma_\varepsilon \quad (5.9)$$

$$-((k_{21})_\varepsilon\nabla c_\varepsilon^e + (k_{22})_\varepsilon\nabla \phi_\varepsilon^e) \cdot \mathbf{n}_s = \mathcal{J}_\varepsilon, \quad x \in \gamma_\varepsilon \quad (5.10)$$

$$-(D_\varepsilon\nabla c_\varepsilon^s) \cdot \mathbf{n}_s = \mathcal{N}_\varepsilon, \quad x \in \gamma_\varepsilon \quad (5.11)$$

$$-(\kappa_\varepsilon\nabla \phi_\varepsilon^s) \cdot \mathbf{n}_s = \mathcal{J}_\varepsilon, \quad x \in \gamma_\varepsilon \quad (5.12)$$

where



- $\mathcal{N}_\varepsilon = \mathcal{N}(c_\varepsilon^e, \phi_\varepsilon^e, \phi_\varepsilon^s, c_\varepsilon^s)$  and
- $\mathcal{J}_\varepsilon = \mathcal{J}(c_\varepsilon^e, \phi_\varepsilon^e, \phi_\varepsilon^s, c_\varepsilon^s)$  and
- $(k_{11})_\varepsilon(x, c_\varepsilon^e) = k_{11}\left(\frac{x}{\varepsilon}, c_\varepsilon^e\right) = k_{11}(y, c_\varepsilon^e) = \chi^e(y)k_{11}^e(c_\varepsilon^e)$ , where  $\chi^e(y)$  is  $Y$ -periodic in  $y$  and therefore  $k_{11}(y, c_\varepsilon^e)$  is also  $Y$ -periodic
- 

$$\chi^e(y) = \begin{cases} 1, & y \in E \\ 0, & y \in S \end{cases}, \quad (5.13)$$

$$\chi^s(y) = 1 - \chi^e(y) \quad (5.14)$$

- $(k_{12})_\varepsilon(x) = k_{12}\left(\frac{x}{\varepsilon}\right) = k_{12}(y) = \chi^e(y)k_{12}^e$ ,  $Y$ -periodic in  $y$
- $(k_{21})_\varepsilon(x, c_\varepsilon^e) = k_{21}\left(\frac{x}{\varepsilon}, c_\varepsilon^e\right) = k_{21}(y, c_\varepsilon^e) = \chi^e(y)k_{21}^e(c_\varepsilon^e)$ ,  $Y$ -periodic in  $y$
- $(k_{22})_\varepsilon(x) = k_{22}\left(\frac{x}{\varepsilon}\right) = k_{22}(y) = \chi^e(y)k_{22}^e$ ,  $Y$ -periodic in  $y$
- $D_\varepsilon(x) = D\left(\frac{x}{\varepsilon}\right) = D(y) = \chi^s(y)D^s$ ,  $Y$ -periodic in the  $y$  variable
- $\kappa_\varepsilon(x) = \kappa\left(\frac{x}{\varepsilon}\right) = \kappa(y) = \chi^s(y)\kappa^s$ ,  $Y$ -periodic in the  $y$  variable

## 5.2 Microscale Solid Equation for the Concentration $c^s$

The diffusion of Lithium ions in the active particles is much slower than the diffusion of ions in the electrolyte. Therefore we do not upscale the equation for the concentration  $c^s$  of Lithium ions in the active particles since the behaviour of the function  $c^s$  can be captured adequately only on the microscale. Thus on the microscale we solve the original microscopic equation for the concentration  $c^s$  of Lithium ions in the active particles given in scale invariant form in terms of the variable  $y \in S$ :

$$\frac{\partial c^s}{\partial t} - \nabla_y \cdot \left( \frac{D^s}{\varepsilon^2} \nabla_y c^s \right) = 0, \quad y \in S \quad (5.15a)$$

$$-\frac{D^s}{\varepsilon^2} \nabla_y c^s \cdot \mathbf{n}_s = \frac{1}{\varepsilon} \mathcal{N}(c_0^e, c^s, \phi_0^e, \phi_0^s), \quad y \in \Gamma \quad (5.15b)$$

, where we have

- $\Gamma$  - the interface boundary between the electrolyte and the particle in the reference periodicity cell  $Y$
- Periodic boundary conditions on  $\partial S \setminus \Gamma$ , i.e. on the boundary of the solid particle where the particles are connected

### 5.3 Asymptotic expansion of the functions $c^\varepsilon$ , $\phi^\varepsilon$ and $\phi^s$

We suppose the following asymptotic expansions for the functions  $c_\varepsilon^e$ ,  $\phi_\varepsilon^e$  and  $\phi_\varepsilon^s$ :

- $c_\varepsilon^e(x, t) = c_0^e(x, t) + \varepsilon c_1^e\left(x, \frac{x}{\varepsilon}, t\right) + \varepsilon^2 c_2^e\left(x, \frac{x}{\varepsilon}, t\right)$
- $\phi_\varepsilon^e(x, t) = \phi_0^e(x, t) + \varepsilon \phi_1^e\left(x, \frac{x}{\varepsilon}, t\right) + \varepsilon^2 \phi_2^e\left(x, \frac{x}{\varepsilon}, t\right)$
- $\phi_\varepsilon^s(x, t) = \phi_0^s(x, t) + \varepsilon \phi_1^s\left(x, \frac{x}{\varepsilon}, t\right) + \varepsilon^2 \phi_2^s\left(x, \frac{x}{\varepsilon}, t\right)$
- $y = \frac{x}{\varepsilon}$
- $\nabla = \nabla_x + \frac{1}{\varepsilon} \nabla_y$

where we assume that the functions  $c_0^e$ ,  $\phi_0^e$  and  $\phi_0^s$  depend only on the macroscopic (slow) variable  $x$  and the functions  $c_1^e$ ,  $c_2^e$ ,  $\phi_1^e$ ,  $\phi_2^e$ ,  $\phi_1^s$ ,  $\phi_2^s$  are  $Y$ -periodic in the  $y = \frac{x}{\varepsilon}$  variable, where  $Y$  is the reference periodicity cell.

For  $y \in Y$ , provided that  $k_{11}^e$  is a smooth function of  $c^e$  in  $E$ , and using Taylor series, for the nonlinear coefficient  $k_{11}(y, c_\varepsilon^e)$  for  $\varepsilon \rightarrow 0$  we obtain:

$$\begin{aligned} k_{11}(y, c_\varepsilon^e) &= k_{11}(y, c_0^e(x, t) + \varepsilon c_1^e(x, y, t)) = \\ &= k_{11}(y, c_0^e) + \varepsilon c_1^e \frac{\partial k_{11}}{\partial c^e}(y, c_0^e) + \varepsilon^2 (c_1^e)^2 \frac{\partial^2 k_{11}}{\partial (c^e)^2}(y, c_0^e) = \\ &= k_{11}(y, c_0^e) + O(\varepsilon) \end{aligned}$$

where

$$\frac{\partial k_{11}}{\partial c^e} = \frac{\partial(\chi^e(y) k_{11}^e(c^e))}{\partial c^e} = \chi^e(y) \frac{\partial k_{11}^e}{\partial c^e} = \begin{cases} \frac{\partial k_{11}^e}{\partial c^e}, & y \in E \\ 0, & y \in S \end{cases}$$

Therefore

$$k_{11}(y, c_\varepsilon^e) = k_{11}(y, c_0^e) + O(\varepsilon)$$

By analogy for the current density  $\mathcal{N}_\varepsilon$  we obtain:

$$\begin{aligned} \mathcal{N}_\varepsilon &= \mathcal{N}(c_\varepsilon^e, c^s, \phi_\varepsilon^e, \phi_\varepsilon^s) = \mathcal{N}(c_0^e + \varepsilon c_1^e, c^s, \phi_0^e + \varepsilon \phi_1^e, \phi_0^s + \varepsilon \phi_1^s) = \\ &= \mathcal{N}(c_0^e, c^s, \phi_0^e, \phi_0^s) + \varepsilon c_1^e \frac{\partial \mathcal{N}}{\partial c^e}(c_0^e, c^s, \phi_0^e, \phi_0^s) + \\ &+ \varepsilon \phi_1^e \frac{\partial \mathcal{N}}{\partial \phi^e}(c_0^e, c^s, \phi_0^e, \phi_0^s) + \varepsilon \phi_1^s \frac{\partial \mathcal{N}}{\partial \phi^s}(c_0^e, c^s, \phi_0^e, \phi_0^s) = \\ &= \mathcal{N}(c_0^e, c^s, \phi_0^e, \phi_0^s) + O(\varepsilon^\alpha) \end{aligned} \tag{5.16}$$

with  $\alpha \geq 1$ .  
 Finally, we obtain

$$k_{11}(y, c_\varepsilon^e) = k_{11}(y, c_0^e) + O(\varepsilon) \quad (5.17)$$

$$k_{21}(y, c_\varepsilon^e) = k_{21}(y, c_0^e) + O(\varepsilon) \quad (5.18)$$

$$\mathcal{N}_\varepsilon = \mathcal{N}(c_\varepsilon^e, c^s, \phi_\varepsilon^e, \phi_\varepsilon^s) = \mathcal{N}(c_0^e, c^s, \phi_0^e, \phi_0^s) + O(\varepsilon^\alpha) \quad (5.19)$$

$$\mathcal{J}_\varepsilon = \mathcal{J}(c_\varepsilon^e, c^s, \phi_\varepsilon^e, \phi_\varepsilon^s) = \mathcal{J}(c_0^e, c^s, \phi_0^e, \phi_0^s) + O(\varepsilon^\alpha) \quad (5.20)$$

We denote

$$\mathcal{N}_0 = \mathcal{N}(c_0^e, c^s, \phi_0^e, \phi_0^s) \quad (5.21)$$

$$\mathcal{J}_0 = \mathcal{J}(c_0^e, c^s, \phi_0^e, \phi_0^s) \quad (5.22)$$

## 5.4 Homogenization of the Interface Conditions

First we show that the total flux over the interfaces is preserved over a change of the total interface surface. A similar idea is applied in [1] and [2] in order for the total flux across the interfaces to be properly scaled.

We use the following notation:

- $\gamma = \gamma_a \cup \gamma_c$  -the interface boundary, where
- $\gamma_a$  - the interface boundary between the anode active particles and the electrolyte
- $\gamma_c$  - the interface boundary between the cathode active particles and the electrolyte

Let us consider the equation for  $\phi^s$  in the cathode where we apply constant current.

$$-\nabla \cdot (\kappa^s \nabla \phi^s) = 0, \quad x \in \Omega_c \quad (5.23)$$

We now integrate both sides of this equation over the domain of the cathode particles and we use the divergence theorem:

$$\begin{aligned} \int_{\Omega_c} -\nabla \cdot (\kappa^s \nabla \phi^s) dx &= 0 \Leftrightarrow \\ \int_{\partial\Omega_c} -\kappa^s \nabla \phi^s \cdot \mathbf{n} ds &= 0 \Leftrightarrow \\ \int_{\gamma_c} \mathcal{J} ds + \int_{\omega_2 \cap \partial\Omega_c} E_2^s ds &= 0 \Leftrightarrow \\ \int_{\gamma_c} \mathcal{J} ds &= - \int_{\omega_2 \cap \partial\Omega_c} E_2^s ds \Leftrightarrow \\ \int_{\gamma_c} \mathcal{J} ds &= -|\omega_2 \cap \partial\Omega_c| E_2^s \end{aligned} \quad (5.24)$$

Since  $E_2^s$  is constant, if we keep the measure of  $\omega_2 \cap \partial\Omega_c$  constant, regardless of the interface surface, the total flux in the cathode  $I = \int_{\gamma_c} \mathcal{J} ds$  is a constant and does not depend on  $\varepsilon$ .

We will show that, indeed, the measure of  $\omega_2 \cap \partial\Omega_c$  is constant with respect to  $\varepsilon$ . In the

case  $\varepsilon = 1$  we have only one particle in each electrode and thus only one periodicity cell which coincides with the whole electrode. Taking into account the type of particles we consider (see Figure 17), it is clear that the intersection of a single particle with the outer battery cell boundary  $\omega_1$  or  $\omega_2$ , is a circle. Let us denote the radius of this circle for  $\varepsilon = 1$  with  $R_1$ . Therefore for the measure  $|\omega_2 \cap \partial\Omega_c|$  we obtain (see Figure 18)

$$S_1 = |\omega_2 \cap \partial\Omega_c| = \pi R_1^2 \quad (5.25)$$

With  $L$  we denote the length of the electrode. Now let us decrease  $\varepsilon$  in such a way that we decrease the length of the periodicity cell twice. This means that in each electrode we have 8 periodicity cells and thus 8 active particles. The side length of each periodicity cell is then  $\frac{L}{2}$ . Let us denote with  $R_2$  the radius of the circle obtained from the intersection of the cathode particle with the outer boundary  $\omega_2$  (see Figure 18). Then the total surface area  $|\omega_2 \cap \partial\Omega_c|$  is

$$S_2 = |\omega_2 \cap \partial\Omega_c| = 4\pi R_2^2 \quad (5.26)$$

Now taking into account that

$$\frac{R_2}{\frac{L}{2}} = \frac{R_1}{L} \quad (5.27)$$

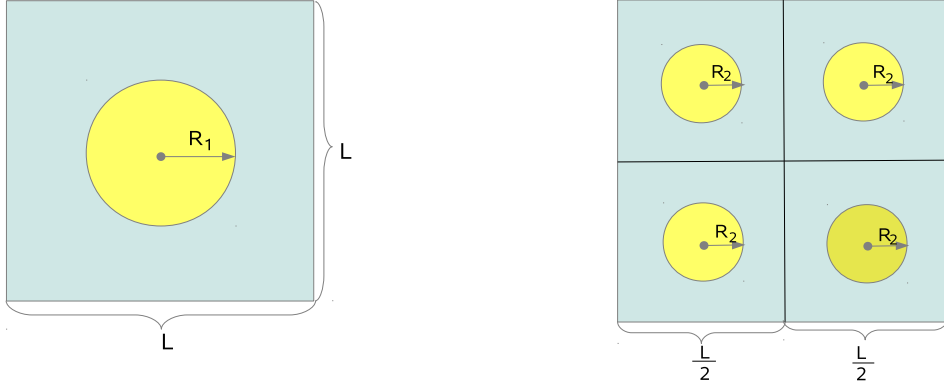
we obtain that

$$R_2 = \frac{R_1}{2} \quad (5.28)$$

and

$$S_2 = 4\pi \frac{R_1^2}{4} = \pi R_1^2 = S_1 \quad (5.29)$$

Consequently we obtain that the measure  $|\omega_2 \cap \partial\Omega_c|$  does not change when we uniformly decrease  $\varepsilon$ .



(a)  $\varepsilon = 1$

(b)  $\varepsilon = 0.5$

Figure 18: Cathode outer boundary

From equation (4.1b) we obtain

$$\begin{aligned}
\int_{\Omega_e} \nabla \cdot \mathbf{J}^e dx &= 0 \Leftrightarrow \\
\int_{\partial\Omega_e} \mathbf{J}^e \cdot \mathbf{n} ds &= 0 \Leftrightarrow \\
\underbrace{\int_{\partial\Omega} \mathbf{J}^e \cdot \mathbf{n} ds}_{=0} + \int_{\gamma} \mathbf{J}^e \cdot \mathbf{n} ds &= 0 \Leftrightarrow \\
-\int_{\gamma} \mathbf{J}^e \cdot \mathbf{n}_s ds &= 0 \Leftrightarrow \\
\int_{\gamma} \mathcal{J} ds &= 0 \Leftrightarrow \\
\int_{\gamma_a} \mathcal{J} ds + \int_{\gamma_c} \mathcal{J} ds &= 0 \Leftrightarrow \\
\int_{\gamma_a} \mathcal{J} ds &= -\int_{\gamma_c} \mathcal{J} ds \tag{5.30}
\end{aligned}$$

From here it follows that since the total flux in the cathode is equal to the total flux in the anode, then the total flux in the anode is also constant with respect to  $\varepsilon$ . We also

have from (4.9) that  $\mathcal{J} = FN$  and consequently we obtain that

$$\int_{\gamma_a} \mathcal{N} ds = \frac{1}{F} \int_{\gamma_a} \mathcal{J} ds \quad (5.31)$$

$$\int_{\gamma_c} \mathcal{N} ds = \frac{1}{F} \int_{\gamma_c} \mathcal{J} ds \quad (5.32)$$

which means that also the total ion flux in each electrode is a constant.

Let  $\varepsilon\Gamma$  be a parametrically defined surface in 3D (the three dimensional Euclidean space). Then we have the following formula for the change of variables:  $x = \varepsilon y$

$$\int_{\varepsilon\Gamma} f(x) ds_x = \varepsilon^2 \int_{\Gamma} g(y) ds_y \quad (5.33)$$

where

$$f(x) = f(x(y)) = f(\varepsilon y) = g(y) \quad (5.34)$$

and the surface  $\varepsilon\Gamma$  transforms into the surface  $\Gamma$  after the change of variables.

Let us denote with  $\varepsilon Y_i$ ,  $i = 1, 2, \dots, M$  the periodic microscale cells where  $\varepsilon Y_i = \varepsilon E_i \cup \varepsilon S_i \cup \varepsilon \Gamma_i$  with  $\varepsilon E_i$  being the electrolyte part of the periodicity cell,  $\varepsilon S_i$ -the solid part, and  $\varepsilon \Gamma_i$ -the interface boundary between the solid and the electrolyte. Then with  $Y_i$  we denote the upscaled periodic cells after the transformation of coordinates  $y = \frac{x}{\varepsilon}$ . Consequently we have that  $Y_i = E_i \cup S_i \cup \Gamma_i$ . For each upscaled periodic cell  $Y_i$  we make the translation  $\tau_i$ :

$$\tau_i : \quad y' = y + \xi_i \quad (5.35)$$

so that

$$Y_i \xrightarrow{\tau_i} Y \quad (5.36)$$

where  $Y$  is the reference periodicity cell, which consists of electrolyte domain  $E$ , active particle domain  $S$  and interface boundary  $\Gamma$ , i.e.  $Y = E \cup S \cup \Gamma$ . We also note that  $\xi_i$  is a constant vector for each periodicity cell  $Y_i$ . Therefore we have that

$$\int_{\Gamma_i} g(y) ds_y = \int_{\Gamma} h(y') ds_{y'} \quad (5.37)$$

where

$$g(y) = g(y(y')) = g(y' - \xi_i) = h(y') \quad (5.38)$$

Let us consider the asymptotic expansion of the function  $c_\varepsilon^e$ :

$$\begin{aligned} c_\varepsilon^e(x) &= c_0^e(x) + \varepsilon c_1^e\left(x, \frac{x}{\varepsilon}\right) + \varepsilon^2 c_2^e\left(x, \frac{x}{\varepsilon}\right) = \\ &= c_0^e(\varepsilon y) + \varepsilon c_1^e(\varepsilon y, y) + \varepsilon^2 c_2^e(\varepsilon y, y) = \\ &= C_0^e(y) + \varepsilon C_1^e(y) + \varepsilon^2 C_2^e(y) = C_\varepsilon^e(y) \end{aligned} \quad (5.39)$$

where we denoted

$$C_0^e(y) = c_0^e(\varepsilon y) \quad (5.40)$$

$$C_1^e(y) = c_1^e(\varepsilon y, y) \quad (5.41)$$

$$C_2^e(y) = c_2^e(\varepsilon y, y) \quad (5.42)$$

By analogy, we obtain similar expressions as (5.39) for the functions  $\phi_\varepsilon^e$  and  $\phi_\varepsilon^s$ . After the change of variables  $y' = y + \xi_i$  which is equivalent to  $y = y' - \xi_i$ , we denote

$$\hat{C}_0^e(y') = C_0^e(y) \quad (5.43)$$

$$\hat{C}_1^e(y') = C_1^e(y) \quad (5.44)$$

$$\hat{C}_2^s(y') = C_2^s(y) \quad (5.45)$$

and we obtain

$$c_\varepsilon^e(x) = \underbrace{C_\varepsilon^e(y) = C_0^e(y) + \varepsilon C_1^e(y) + \varepsilon^2 C_2^e(y)}_{\hat{C}_\varepsilon^e(y')} = \underbrace{\hat{C}_0^e(y') + \varepsilon \hat{C}_1^e(y') + \varepsilon^2 \hat{C}_2^e(y')}_{\hat{C}_\varepsilon^e(y')} \quad (5.46)$$

or equivalently

$$c_\varepsilon^e(x) = C_\varepsilon^e(y) = \hat{C}_\varepsilon^e(y') \quad (5.47)$$

By analogy, for the functions  $\phi_\varepsilon^e(x)$  and  $\phi_\varepsilon^s(x)$  we obtain

$$\phi_\varepsilon^e(x) = \Phi_\varepsilon^e(y) = \hat{\Phi}_\varepsilon^e(y') \quad (5.48)$$

$$\phi_\varepsilon^s(x) = \Phi_\varepsilon^s(y) = \hat{\Phi}_\varepsilon^s(y') \quad (5.49)$$

For the concentration  $c^s$  of ions in the particles we have

$$c^s(x) = C^s(y) = \hat{C}^s(y') \quad (5.50)$$

For the current density we use the following notation:

$$\mathcal{N}_\varepsilon = \mathcal{N}(c_\varepsilon^e(x), c^s(x), \phi_\varepsilon^e(x), \phi_\varepsilon^s(x)) = f_\varepsilon(x) \quad (5.51)$$

$$(5.52)$$

Therefore after the subsequent changes of variables  $x = \varepsilon y$  and  $y' = y + \xi_i$  we obtain

$$\begin{aligned} \mathcal{N}_\varepsilon &= \mathcal{N}(c_\varepsilon^e(x), c^s(x), \phi_\varepsilon^e(x), \phi_\varepsilon^s(x)) = f_\varepsilon(x) = \\ &= \underbrace{\mathcal{N}(C_\varepsilon^e(y), C^s(y), \Phi_\varepsilon^e(y), \Phi_\varepsilon^s(y))}_{g_\varepsilon(y)} = \\ &= \underbrace{\mathcal{N}(\hat{C}_\varepsilon^e(y'), \hat{C}^s(y'), \hat{\Phi}_\varepsilon^e(y'), \hat{\Phi}_\varepsilon^s(y'))}_{h_\varepsilon(y')} \end{aligned} \quad (5.53)$$

where we denoted

$$\begin{aligned} g_\varepsilon(y) &= \mathcal{N}(C_\varepsilon^e(y), C^s(y), \Phi_\varepsilon^e(y), \Phi_\varepsilon^s(y)) \\ h_\varepsilon(y') &= \mathcal{N}(\hat{C}_\varepsilon^e(y'), \hat{C}^s(y'), \hat{\Phi}_\varepsilon^e(y'), \hat{\Phi}_\varepsilon^s(y')) \end{aligned} \quad (5.54)$$

We denote with  $\varepsilon\Gamma_i$  the interface boundary for each periodicity cell  $\varepsilon Y_i$  and with  $\varepsilon\Gamma = \sum_{i=1}^M \varepsilon\Gamma_i$  the whole interface boundary in the electrode (if we follow the already

introduced notation for the interface boundary, namely  $\gamma = \gamma_a \cup \gamma_c$ , and taking into account the dependence on  $\varepsilon$ , we should use here  $\gamma_a^\varepsilon$  and  $\gamma_c^\varepsilon$ , but we use instead the  $\varepsilon\Gamma$  notation for simplicity). The number of all the microscopic periodicity cells in the electrode ( which is a cube with length of the side  $L$ , or a parallelepiped with a characteristic length of the sides  $L$ , then the total number of periodicity cells is of order  $\frac{1}{\varepsilon^3} = \left(\frac{L}{l}\right)^3$  ) is

$$M \sim \left(\frac{L}{l}\right)^3 = \frac{1}{\varepsilon^3}. \text{ This means that } M \sim O\left(\frac{1}{\varepsilon^3}\right).$$

We showed that the total flux  $I$  across the whole interface boundary must be preserved, i.e. must be the same, no matter how many active particles we have in the electrode (provided that we impose the same Neumann and Dirichlet boundary conditions on the outer cathode and anode boundaries). This is due to the fact that all the outer boundaries of the battery cell are insulated except for the cathode and anode boundaries  $\omega_1$  and  $\omega_2$  where we apply constant potential and constant current respectively. Therefore the total flux across the interface must be the same constant if we have one, two, or thousands of particles, i.e the total flux must not depend on  $\varepsilon$ .

Then for the total flux across the whole interface boundary  $\varepsilon\Gamma$  in the case of multiple active particles, we obtain

$$\begin{aligned} I &= \int_{\varepsilon\Gamma} -((k_{11})_\varepsilon \nabla c_\varepsilon^e + (k_{12})_\varepsilon \nabla \phi_\varepsilon^e) \cdot \mathbf{n}_s ds_x = \int_{\varepsilon\Gamma} \mathcal{N}_\varepsilon ds_x = \\ &= \sum_{i=1}^M \int_{\varepsilon\Gamma_i} \mathcal{N}_\varepsilon ds_x = \sum_{i=1}^M \int_{\varepsilon\Gamma_i} \mathcal{N}(c_\varepsilon^e(x), c^s(x), \phi_\varepsilon^e(x), \phi_\varepsilon^s(x)) ds_x = \\ &= \sum_{i=1}^M \int_{\varepsilon\Gamma_i} f_\varepsilon(x) ds_x = \sum_{i=1}^M \varepsilon^2 \int_{\Gamma_i} g_\varepsilon(y) ds_y = \\ &= \sum_{i=1}^M \varepsilon^2 \left( \int_{\Gamma_i} g_\varepsilon(y) ds_y \right) = \sum_{i=1}^M \varepsilon^2 \left( \int_{\Gamma} h_\varepsilon(y') ds_{y'} \right) = \\ &= \sum_{i=1}^M \left( \varepsilon^2 \int_{\Gamma} h_\varepsilon(y') ds_{y'} \right) = \frac{1}{\varepsilon^3} \left( \varepsilon^2 \int_{\Gamma} h_\varepsilon(y') ds_{y'} \right) = \\ &= \varepsilon^{-1} \int_{\Gamma} h_\varepsilon(y') ds_{y'} \end{aligned} \tag{5.55}$$

From the latter it follows that the total flux  $I$  does not depend on  $\varepsilon$  if and only if

$$h_\varepsilon(y') = O(\varepsilon) \tag{5.56}$$

But we have that

$$\mathcal{N}_\varepsilon = \mathcal{N}(c_\varepsilon^e(x), c^s(x), \phi_\varepsilon^e(x), \phi_\varepsilon^s(x)) = f_\varepsilon(x) = g_\varepsilon(y) = h_\varepsilon(y')$$

and consequently

$$\mathcal{N}_\varepsilon = O(\varepsilon) \tag{5.57}$$



From (5.19) it follows that

$$\mathcal{N}_0 = O(\varepsilon) \quad (5.58)$$

(we have  $\mathcal{N}_\varepsilon = \mathcal{N}(c_0^e, c^s, \phi_0^e, \phi_0^s) + O(\varepsilon^\alpha) = O(\varepsilon)(1 + O(\varepsilon^{\alpha-1})) = O(\varepsilon)$ ) Thus we obtained that the current densities  $\mathcal{N}_\varepsilon$  and  $\mathcal{J}_\varepsilon$  must be of order  $\varepsilon$ . On the other hand, from physical considerations and from the numerical results from the full microscopic simulations [11] we also show experimentally that  $\mathcal{N}_\varepsilon$  and  $\mathcal{J}_\varepsilon$  are of order  $\varepsilon$  implicitly, i.e. the current density decreases with rate  $\varepsilon$  when we increase the number of particles.

Finally, for the interface conditions in each electrode we obtain:

$$-((k_{11})_\varepsilon \nabla c_\varepsilon^e + (k_{12})_\varepsilon \nabla \phi_\varepsilon^e) \cdot \mathbf{n}_s = \mathcal{N}_\varepsilon, \quad x \in \varepsilon\Gamma \quad (5.59)$$

$$-((k_{21})_\varepsilon \nabla c_\varepsilon^e + (k_{22})_\varepsilon \nabla \phi_\varepsilon^e) \cdot \mathbf{n}_s = \mathcal{J}_\varepsilon, \quad x \in \varepsilon\Gamma \quad (5.60)$$

$$-(D^s \nabla c^s) \cdot \mathbf{n}_s = \mathcal{N}_0, \quad x \in \Gamma \quad (5.61)$$

$$-(\kappa_\varepsilon \nabla \phi_\varepsilon^s) \cdot \mathbf{n}_s = \mathcal{J}_\varepsilon, \quad x \in \varepsilon\Gamma \quad (5.62)$$

Thus for the homogenization of the interface conditions we obtain

$$\begin{aligned} \mathcal{N}_\varepsilon &= \mathbf{N}_\varepsilon^e \cdot \mathbf{n}_s = -\{k_{11}(y, c_\varepsilon^e) \nabla c_\varepsilon^e + k_{12}(y) \nabla \phi_\varepsilon^e\} \cdot \mathbf{n}_s = \\ &= -\left\{k_{11}(y, c_0^e) \left(\nabla_x + \frac{1}{\varepsilon} \nabla_y\right) (c_0^e + \varepsilon c_1^e + \varepsilon^2 c_2^e) + \right. \\ &\quad \left. + k_{12}(y) \left(\nabla_x + \frac{1}{\varepsilon} \nabla_y\right) (\phi_0^e + \varepsilon \phi_1^e + \varepsilon^2 \phi_2^e)\right\} \cdot \mathbf{n}_s = \\ &= -\left\{\frac{1}{\varepsilon} [k_{11}(y, c_0^e) \nabla_y c_0^e + k_{12}(y) \nabla_y \phi_0^e] + \right. \\ &\quad + \varepsilon^0 [k_{11}(y, c_0^e) (\nabla_x c_0^e + \nabla_y c_1^e) + k_{12}(y) (\nabla_x \phi_0^e + \nabla_y \phi_1^e)] + \\ &\quad + \varepsilon [k_{11}(y, c_0^e) (\nabla_x c_1^e + \nabla_y c_2^e) + k_{12}(y) (\nabla_x \phi_1^e + \nabla_y \phi_2^e)] + \\ &\quad \left. + \varepsilon^2[\dots]\right\} \cdot \mathbf{n}_s \end{aligned} \quad (5.63)$$

which is equivalent to

$$\begin{aligned} \frac{1}{\varepsilon} \mathcal{N}_\varepsilon &= -\left[ \frac{1}{\varepsilon^2} (k_{11}(y, c_0^e) \nabla_y c_0^e + k_{12}(y) \nabla_y \phi_0^e) + \right. \\ &\quad + \frac{1}{\varepsilon} (k_{11}(y, c_0^e) (\nabla_x c_0^e + \nabla_y c_1^e) + k_{12}(y) (\nabla_x \phi_0^e + \nabla_y \phi_1^e)) + \\ &\quad + \varepsilon^0 (k_{11}(y, c_0^e) (\nabla_x c_1^e + \nabla_y c_2^e) + k_{12}(y) (\nabla_x \phi_1^e + \nabla_y \phi_2^e)) + \\ &\quad \left. + \varepsilon(\dots) \right] \cdot \mathbf{n}_s \end{aligned} \quad (5.64)$$

Now taking into account that  $\mathcal{N}_\varepsilon = O(\varepsilon) = \mathcal{N}(c_0^e, c^s, \phi_0^e, \phi_0^s) + O(\varepsilon^2)$ , and consequently  $\mathcal{N}(c_0^e, c^s, \phi_0^e, \phi_0^s) = O(\varepsilon)$ , it follows that  $\frac{1}{\varepsilon} \mathcal{N}_0 = O(1)$ . Then, by grouping equal powers of

$\varepsilon$ , we obtain

$$\begin{aligned}
\varepsilon^{-2} : \quad 0 &= \left[ k_{11}(y, c_0^e) \underbrace{\nabla_y c_0^e}_{=0} + k_{12}(y) \underbrace{\nabla_y \phi_0^e}_{=0} \right] \cdot \mathbf{n}_s \iff 0 = 0 \\
\varepsilon^{-1} : \quad 0 &= [k_{11}(y, c_0^e) (\nabla_x c_0^e + \nabla_y c_1^e) + k_{12}(y) (\nabla_x \phi_0^e + \nabla_y \phi_1^e)] \cdot \mathbf{n}_s \\
\varepsilon^0 : \quad \frac{1}{\varepsilon} \mathcal{N}(c_0^e, c^s, \phi_0^e, \phi_0^s) &= \\
&= - [k_{11}(y, c_0^e) \nabla_x c_1^e + k_{11}(y, c_0^e) \nabla_y c_2^e + k_{12}(y) \nabla_x \phi_1^e + k_{12}(y) \nabla_y \phi_2^e] \cdot \mathbf{n}_s \quad (5.65)
\end{aligned}$$

where we account for the fact that the functions  $c_0^e$  and  $\phi_0^e$  depend only on  $x$  and do not depend on  $y$ . By analogy, from  $\mathbf{J}_\varepsilon^e \cdot \mathbf{n}_s = \mathcal{J}_\varepsilon$  we obtain:

$$\begin{aligned}
\varepsilon^{-2} : \quad 0 &= \left[ k_{21}(y, c_0^e) \underbrace{\nabla_y c_0^e}_{=0} + k_{22}(y) \underbrace{\nabla_y \phi_0^e}_{=0} \right] \cdot \mathbf{n}_s \iff 0 = 0 \\
\varepsilon^{-1} : \quad 0 &= [k_{21}(y, c_0^e) (\nabla_x c_0^e + \nabla_y c_1^e) + k_{22}(y) (\nabla_x \phi_0^e + \nabla_y \phi_1^e)] \cdot \mathbf{n}_s \\
\varepsilon^0 : \quad \frac{1}{\varepsilon} \mathcal{J}(c_0^e, c^s, \phi_0^e, \phi_0^s) &= \\
&= - [k_{21}(y, c_0^e) \nabla_x c_1^e + k_{21}(y, c_0^e) \nabla_y c_2^e + k_{22}(y) \nabla_x \phi_1^e + k_{22}(y) \nabla_y \phi_2^e] \cdot \mathbf{n}_s \quad (5.66)
\end{aligned}$$

## 5.5 Homogenization of the Electrolyte Phase PDEs

For the time derivative  $\frac{\partial (\chi_\varepsilon^e(x) c_\varepsilon^e)}{\partial t}$  we take the zero order approximation  $\frac{\partial (\chi_\varepsilon^e(x) c_0)}{\partial t}$ , i.e.  $\frac{\partial (\chi_\varepsilon^e(x) c_\varepsilon^e)}{\partial t} = \frac{\partial (\chi^e(y) \partial c_0)}{\partial t} + O(\varepsilon)$ . We have that  $y \in Y = E \cup S$  and  $x \in \Omega$ .

Therefore for equation (5.5a) we obtain:

$$\begin{aligned}
\frac{\partial (\chi^\varepsilon(y)c_0)}{\partial t} &= \nabla \cdot ((k_{11})_\varepsilon(x, c_\varepsilon^e) \nabla c_\varepsilon^e + (k_{12})_\varepsilon(x) \nabla \phi_\varepsilon^e) = \\
&= \left( \nabla_x + \frac{1}{\varepsilon} \nabla_y \right) \cdot \left[ k_{11}(y, c_0^e) \left( \nabla_x + \frac{1}{\varepsilon} \nabla_y \right) (c_0^e(x, t) + \varepsilon c_1^e(x, y, t) + \varepsilon^2 c_2^e(x, y, t)) + \right. \\
&+ k_{12}(y) \left( \nabla_x + \frac{1}{\varepsilon} \nabla_y \right) (\phi_0^e(x, t) + \varepsilon \phi_1^e(x, y, t) + \varepsilon^2 \phi_2^e(x, y, t)) \left. \right] = \\
&= \left( \nabla_x + \frac{1}{\varepsilon} \nabla_y \right) \cdot \left[ k_{11}(y, c_0^e) \nabla_x c_0^e + \varepsilon k_{11}(y, c_0^e) \nabla_x c_1^e + \varepsilon^2 k_{11}(y, c_0^e) \nabla_x c_2^e + \frac{1}{\varepsilon} k_{11}(y, c_0^e) \nabla_y c_0^e + \right. \\
&+ k_{11}(y, c_0^e) \nabla_y c_1^e + \varepsilon k_{11}(y, c_0^e) \nabla_y c_2^e + k_{12}(y) \nabla_x \phi_0^e + \varepsilon k_{12}(y) \nabla_x \phi_1^e + \varepsilon^2 k_{12}(y) \nabla_x \phi_2^e + \\
&+ \frac{1}{\varepsilon} k_{12}(y) \nabla_y \phi_0^e + k_{12}(y) \nabla_y \phi_1^e + \varepsilon k_{12}(y) \nabla_y \phi_2^e \left. \right] = \\
&= \left( \nabla_x + \frac{1}{\varepsilon} \nabla_y \right) \cdot \{ k_{11}(y, c_0^e) (\nabla_x c_0^e + \nabla_y c_1^e) + k_{12}(y) (\nabla_x \phi_0^e + \nabla_y \phi_1^e) + \\
&+ \varepsilon [k_{11}(y, c_0^e) (\nabla_x c_1^e + \nabla_y c_2^e) + k_{12}(y) (\nabla_x \phi_1^e + \nabla_y \phi_2^e)] + \\
&+ \varepsilon^2 (k_{11}(y, c_0^e) \nabla_x c_2^e + k_{12}(y) \nabla_x \phi_2^e) + \frac{1}{\varepsilon} (k_{11}(y, c_0^e) \nabla_y c_0^e + k_{12}(y) \nabla_y \phi_0^e) \} = \\
&= \frac{1}{\varepsilon^2} \nabla_y \cdot \{ k_{11}(y, c_0^e) \nabla_y c_0^e + k_{12}(y) \nabla_y \phi_0^e \} + \\
&+ \frac{1}{\varepsilon} \{ \nabla_x \cdot (k_{11}(y, c_0^e) \nabla_y c_0^e + k_{12}(y) \nabla_y \phi_0^e) + \\
&+ \nabla_y \cdot (k_{11}(y, c_0^e) \nabla_x c_0^e + k_{11}(y, c_0^e) \nabla_y c_1^e + k_{12}(y) \nabla_x \phi_0^e + k_{12}(y) \nabla_y \phi_1^e) \} + \\
&+ \varepsilon^0 \{ \nabla_x \cdot [k_{11}(y, c_0^e) \nabla_x c_0^e + k_{11}(y, c_0^e) \nabla_y c_1^e + k_{12}(y) \nabla_x \phi_0^e + k_{12}(y) \nabla_y \phi_1^e] + \\
&+ \nabla_y \cdot [k_{11}(y, c_0^e) \nabla_x c_1^e + k_{11}(y, c_0^e) \nabla_y c_2^e + k_{12}(y) \nabla_x \phi_1^e + k_{12}(y) \nabla_y \phi_2^e] \} + \\
&+ \varepsilon \{ \nabla_x \cdot (k_{11}(y, c_0^e) \nabla_x c_1^e + k_{11}(y, c_0^e) \nabla_y c_2^e + k_{12}(y) \nabla_x \phi_1^e + k_{12}(y) \nabla_y \phi_2^e) + \\
&+ \nabla_y \cdot (k_{11}(y, c_0^e) \nabla_x c_2^e + k_{12}(y) \nabla_x \phi_2^e) \} + \\
&+ \varepsilon^2 \nabla_x \cdot \{ k_{11}(y, c_0^e) \nabla_x c_2^e + k_{12}(y) \nabla_x \phi_2^e \}
\end{aligned} \tag{5.67}$$

Therefore from the equal powers of  $\varepsilon$  we obtain:

$$\varepsilon^{-2} : \quad \nabla_y \cdot \left( k_{11}(y, c_0^e) \underbrace{\nabla_y c_0^e}_{=0} + k_{12}(y) \underbrace{\nabla_y \phi_0^e}_{=0} \right) = 0 \iff 0 = 0 \quad (5.68)$$

$$\begin{aligned} \varepsilon^{-1} : \quad & \nabla_x \cdot \left( k_{11}(y, c_0^e) \underbrace{\nabla_y c_0^e}_{=0} + k_{12}(y) \underbrace{\nabla_y \phi_0^e}_{=0} \right) + \\ & + \nabla_y \cdot (k_{11}(y, c_0^e) \nabla_x c_0^e + k_{11}(y, c_0^e) \nabla_y c_1^e + k_{12}(y) \nabla_x \phi_0^e + k_{12}(y) \nabla_y \phi_1^e) = 0 \end{aligned} \quad (5.69)$$

$$\begin{aligned} \varepsilon^0 : \quad & \chi^e(y) \frac{\partial c_0^e}{\partial t} = \nabla_x \cdot [k_{11}(y, c_0^e) \nabla_x c_0^e + k_{11}(y, c_0^e) \nabla_y c_1^e + k_{12}(y) \nabla_x \phi_0^e + k_{12}(y) \nabla_y \phi_1^e] + \\ & + \nabla_y \cdot [k_{11}(y, c_0^e) \nabla_x c_1^e + k_{11}(y, c_0^e) \nabla_y c_2^e + k_{12}(y) \nabla_x \phi_1^e + k_{12}(y) \nabla_y \phi_2^e] \end{aligned} \quad (5.70)$$

We have analogous result for the second partial differential equation from the electrolyte system of equations:

$$\varepsilon^{-2} : \quad \nabla_y \cdot \left( k_{21}(y, c_0^e) \underbrace{\nabla_y c_0^e}_{=0} + k_{22}(y) \underbrace{\nabla_y \phi_0^e}_{=0} \right) = 0 \iff 0 = 0 \quad (5.71)$$

$$\begin{aligned} \varepsilon^{-1} : \quad & \nabla_x \cdot \left( k_{21}(y, c_0^e) \underbrace{\nabla_y c_0^e}_{=0} + k_{22}(y) \underbrace{\nabla_y \phi_0^e}_{=0} \right) + \\ & + \nabla_y \cdot (k_{21}(y, c_0^e) \nabla_x c_0^e + k_{21}(y, c_0^e) \nabla_y c_1^e + k_{22}(y) \nabla_x \phi_0^e + k_{22}(y) \nabla_y \phi_1^e) = 0 \end{aligned} \quad (5.72)$$

$$\begin{aligned} \varepsilon^0 : \quad & 0 = \nabla_x \cdot [k_{21}(y, c_0^e) \nabla_x c_0^e + k_{21}(y, c_0^e) \nabla_y c_1^e + k_{22}(y) \nabla_x \phi_0^e + k_{22}(y) \nabla_y \phi_1^e] + \\ & + \nabla_y \cdot [k_{21}(y, c_0^e) \nabla_x c_1^e + k_{21}(y, c_0^e) \nabla_y c_2^e + k_{22}(y) \nabla_x \phi_1^e + k_{22}(y) \nabla_y \phi_2^e] \end{aligned} \quad (5.73)$$

### 5.5.1 Order $\varepsilon^{-1}$ : Derivation of the Auxiliary Cell Problems

We have the following system of equations for  $y \in Y$  and  $x \in \Omega$

$$\nabla_y \cdot (k_{11}(y, c_0^e) \nabla_x c_0^e + k_{11}(y, c_0^e) \nabla_y c_1^e + k_{12}(y) \nabla_x \phi_0^e + k_{12}(y) \nabla_y \phi_1^e) = 0 \quad (5.74a)$$

$$\nabla_y \cdot (k_{21}(y, c_0^e) \nabla_x c_0^e + k_{21}(y, c_0^e) \nabla_y c_1^e + k_{22}(y) \nabla_x \phi_0^e + k_{22}(y) \nabla_y \phi_1^e) = 0 \quad (5.74b)$$

which is equivalent to

$$\nabla_y \cdot (k_{11}(y, c_0^e) \nabla_y c_1^e + k_{12}(y) \nabla_y \phi_1^e) = -\nabla_y \cdot (k_{11}(y, c_0^e) \nabla_x c_0^e + k_{12}(y) \nabla_x \phi_0^e) \quad (5.75a)$$

$$\nabla_y \cdot (k_{21}(y, c_0^e) \nabla_y c_1^e + k_{22}(y) \nabla_y \phi_1^e) = -\nabla_y \cdot (k_{21}(y, c_0^e) \nabla_x c_0^e + k_{22}(y) \nabla_x \phi_0^e) \quad (5.75b)$$

with the following interface conditions:

$$(k_{11}(y, c_0^e) \nabla_y c_1^e + k_{12}(y) \nabla_y \phi_1^e) \cdot \mathbf{n}_s = - (k_{11}(y, c_0^e) \nabla_x c_0^e + k_{12}(y) \nabla_x \phi_0^e) \cdot \mathbf{n}_s \quad (5.76a)$$

$$(k_{21}(y, c_0^e) \nabla_y c_1^e + k_{22}(y) \nabla_y \phi_1^e) \cdot \mathbf{n}_s = - (k_{21}(y, c_0^e) \nabla_x c_0^e + k_{22}(y) \nabla_x \phi_0^e) \cdot \mathbf{n}_s \quad (5.76b)$$

We introduce the following notation for system (5.75) of PDEs:

$$\nabla_y \cdot (K(y, x) \nabla_y U_1) = - \nabla_y \cdot (K(y, x) \nabla_x U_0) \quad (5.77)$$

where we denote

$$K = \begin{pmatrix} k_{11} & k_{12} \\ k_{21} & k_{22} \end{pmatrix}, \quad U_1 = \begin{pmatrix} c_1^e(x, y) \\ \phi_1^e(x, y) \end{pmatrix}, \quad U_0 = \begin{pmatrix} c_0^e(x) \\ \phi_0^e(x) \end{pmatrix},$$

$$\nabla_y U_1 = \begin{pmatrix} \nabla_y c_1^e \\ \nabla_y \phi_1^e \end{pmatrix}, \quad \nabla_x U_0 = \begin{pmatrix} \nabla_x c_0^e \\ \nabla_x \phi_0^e \end{pmatrix}$$

### • Some Notations

- Divergence of a vector whose elements are vectors

$$\nabla_y \cdot \begin{pmatrix} v_1(y) \\ v_2(y) \end{pmatrix} = \begin{pmatrix} \nabla_y \cdot v_1 \\ \nabla_y \cdot v_2 \end{pmatrix}$$

- Scalar product of matrix and vector

$$A \cdot \mathbf{v} = \begin{pmatrix} a_{11} & \dots & a_{1n} \\ \dots & \dots & \dots \\ a_{n1} & \dots & a_{nn} \end{pmatrix} \cdot \mathbf{v} = \begin{pmatrix} (a_{11}, \dots, a_{1n}) \cdot \mathbf{v} \\ \dots \\ (a_{n1}, \dots, a_{nn}) \cdot \mathbf{v} \end{pmatrix}$$

- Divergence of a matrix

$$\nabla_y \cdot A = \nabla_y \cdot \begin{pmatrix} a_{11} & \dots & a_{1n} \\ \dots & \dots & \dots \\ a_{n1} & \dots & a_{nn} \end{pmatrix} = \begin{pmatrix} \nabla_y \cdot (a_{11}, \dots, a_{1n}) \\ \dots \\ \nabla_y \cdot (a_{n1}, \dots, a_{nn}) \end{pmatrix}$$

Let  $w(y)$  be a matrix  $2 \times 3$  whose elements are functions of  $y$ , i.e.

$$w(y) = \begin{pmatrix} w_1(y) \\ w_2(y) \end{pmatrix} = \begin{pmatrix} w_{11}(y) & w_{12}(y) & w_{13}(y) \\ w_{21}(y) & w_{22}(y) & w_{23}(y) \end{pmatrix}$$

where

$$w_1(y) = (w_{11}(y), w_{12}(y), w_{13}(y))$$

$$w_2(y) = (w_{21}(y), w_{22}(y), w_{23}(y))$$

Then we define the scalar product

$$\nabla_x U_0 \cdot w(y) = \begin{pmatrix} \nabla_x c_0^e \\ \nabla_x \phi_0^e \end{pmatrix} \cdot \begin{pmatrix} w_1(y) \\ w_2(y) \end{pmatrix} = \begin{pmatrix} \nabla_x c_0^e \cdot w_1 \\ \nabla_x \phi_0^e \cdot w_2 \end{pmatrix}$$

Now by analogy with the scalar case, from the equation  $\nabla_y \cdot (K \nabla_y U_1) = -\nabla_y \cdot (K \nabla_x U_0)$  we look for the solution  $U_1(x, y)$  of this equation in the following form

$$U_1(x, y) = \nabla_x U_0 \cdot w(y) \quad (5.78)$$

Now by definition we have that

$$\nabla_y U_1 = \begin{pmatrix} \nabla_y (\nabla_x c_0^e \cdot w_1) \\ \nabla_y (\nabla_x \phi_0^e \cdot w_2) \end{pmatrix} = \begin{pmatrix} \sum_{i=1}^3 \frac{\partial c_0^e}{\partial x_i} \nabla_y w_{1i} \\ \sum_{i=1}^3 \frac{\partial \phi_0^e}{\partial x_i} \nabla_y w_{2i} \end{pmatrix}$$

We denote

$$a_i = \frac{\partial c_0^e}{\partial x_i} \nabla_y w_{1i}$$

$$b_i = \frac{\partial \phi_0^e}{\partial x_i} \nabla_y w_{2i}$$

Therefore

$$\nabla_y U_1 = \begin{pmatrix} \sum_{i=1}^3 a_i \\ \sum_{i=1}^3 b_i \end{pmatrix}$$

Then we have that

$$\begin{aligned} K \nabla_y U_1 &= K \begin{pmatrix} \sum_{i=1}^3 a_i \\ \sum_{i=1}^3 b_i \end{pmatrix} = \sum_{i=1}^3 K \begin{pmatrix} a_i \\ b_i \end{pmatrix} = \sum_{i=1}^3 \begin{pmatrix} k_{11} & k_{12} \\ k_{21} & k_{22} \end{pmatrix} \begin{pmatrix} a_i \\ b_i \end{pmatrix} = \\ &= \sum_{i=1}^3 \begin{pmatrix} k_{11} a_i + k_{12} b_i \\ k_{21} a_i + k_{22} b_i \end{pmatrix} = \sum_{i=1}^3 K V_i \end{aligned}$$

where

$$V_i = \begin{pmatrix} a_i \\ b_i \end{pmatrix}$$

Now, after we substitute  $U_1(x, y)$  with  $\nabla_x U_0 \cdot w(y)$  in the equation  $\nabla_y \cdot (K(y, x) \nabla_y U_1) = -\nabla_y \cdot (K(y, x) \nabla_x U_0)$  we obtain the following equality which must be satisfied for each  $x \in \Omega$ :

$$\sum_{i=1}^3 \nabla_y \cdot (K(y, x) V_i) = -\nabla_y \cdot (K(y, x) \nabla_x U_0)$$

Since

$$\begin{aligned} k_{11}(y, c_0) &= \chi^e(y)k_{11}^e(c_0^e), & k_{12}(y) &= \chi^e(y)k_{12}^e \\ k_{21}(y, c_0) &= \chi^e(y)k_{21}^e(c_0^e), & k_{22}(y) &= \chi^e(y)k_{22}^e \end{aligned}$$

we have that  $K(y, x) = \chi^e(y)K^e(x)$ , and for  $y \in S$  we have that  $\chi^e(y) = 0$ , and  $\chi^e(y) = 1$  for  $y \in E$ . Hence for  $y \in E$  we have that  $K(y, x) = K^e(x)$  and consequently  $-\nabla_y \cdot (K^e(x)\nabla_x U_0(x)) = 0$ . Therefore the equality

$$\sum_{i=1}^3 \nabla_y \cdot (K(y, x)V_i) = -\nabla_y \cdot (K(y, x)\nabla_x U_0)$$

which must be true for each  $x \in \Omega$ , for  $y \in E$  is equivalent to

$$\sum_{i=1}^3 \nabla_y \cdot (K^e(x)V_i) = -\nabla_y \cdot (K^e(x)\nabla_x U_0), \quad y \in E$$

is equivalent to

$$\sum_{i=1}^3 \nabla_y \cdot (K^e(x)V_i) = 0, \quad y \in E$$

$$\begin{aligned} V_i &= \begin{pmatrix} a_i \\ b_i \end{pmatrix} = \begin{pmatrix} \frac{\partial c_0^e}{\partial x_i} \nabla_y w_{1i} \\ \frac{\partial \phi_0^e}{\partial x_i} \nabla_y w_{2i} \end{pmatrix} = \\ &= \underbrace{\begin{pmatrix} \frac{\partial c_0^e}{\partial x_i}(x) & 0 \\ 0 & \frac{\partial \phi_0^e}{\partial x_i}(x) \end{pmatrix}}_{=C_i} \begin{pmatrix} \nabla_y w_{1i} \\ \nabla_y w_{2i} \end{pmatrix} = C_i \begin{pmatrix} \nabla_y w_{1i} \\ \nabla_y w_{2i} \end{pmatrix} \end{aligned}$$

From here it follows that for the equality  $\sum_{i=1}^3 \nabla_y \cdot (K^e(x)V_i) = 0$ ,  $y \in E$  we obtain:

$$\sum_{i=1}^3 \nabla_y \cdot \left( K^e(x)C_i(x) \begin{pmatrix} \nabla_y w_{1i} \\ \nabla_y w_{2i} \end{pmatrix} \right) = 0, \quad y \in E$$

We denote

$$A(x) = (a_{ij})_{i,j=1}^2 = K^e(x)C_i(x)$$

Then

$$A(x) \begin{pmatrix} \nabla_y w_{1i} \\ \nabla_y w_{2i} \end{pmatrix} = \begin{pmatrix} a_{11}\nabla_y w_{1i} + a_{12}\nabla_y w_{2i} \\ a_{21}\nabla_y w_{1i} + a_{22}\nabla_y w_{2i} \end{pmatrix}$$

Therefore by definition we have that

$$\nabla_y \cdot \begin{pmatrix} a_{11} \nabla_y w_{1i} + a_{12} \nabla_y w_{2i} \\ a_{21} \nabla_y w_{1i} + a_{22} \nabla_y w_{2i} \end{pmatrix} = \begin{pmatrix} \nabla_y \cdot (a_{11} \nabla_y w_{1i} + a_{12} \nabla_y w_{2i}) \\ \nabla_y \cdot (a_{21} \nabla_y w_{1i} + a_{22} \nabla_y w_{2i}) \end{pmatrix}$$

Hence the equality

$$\sum_{i=1}^3 \nabla_y \cdot \left( K^e(x) C_i(x) \begin{pmatrix} \nabla_y w_{1i} \\ \nabla_y w_{2i} \end{pmatrix} \right) = \vec{0}, \quad y \in E$$

which is equivalent to

$$\sum_{i=1}^3 \nabla_y \cdot \left( A(x) \begin{pmatrix} \nabla_y w_{1i} \\ \nabla_y w_{2i} \end{pmatrix} \right) = \vec{0}, \quad y \in E$$

becomes

$$\sum_{i=1}^3 \begin{pmatrix} \nabla_y \cdot (a_{11} \nabla_y w_{1i} + a_{12} \nabla_y w_{2i}) \\ \nabla_y \cdot (a_{21} \nabla_y w_{1i} + a_{22} \nabla_y w_{2i}) \end{pmatrix} = \vec{0}, \quad y \in E$$

By definition, the latter is equivalent to

$$\begin{cases} \sum_{i=1}^3 \nabla_y \cdot (a_{11}(x) \nabla_y w_{1i} + a_{12}(x) \nabla_y w_{2i}) = 0, & y \in E \\ \sum_{i=1}^3 \nabla_y \cdot (a_{21}(x) \nabla_y w_{1i} + a_{22}(x) \nabla_y w_{2i}) = 0, & y \in E \end{cases}$$

which is equivalent to

$$\begin{cases} \sum_{i=1}^3 \{a_{11}(x) \nabla_y \cdot (\nabla_y w_{1i}) + a_{12}(x) \nabla_y \cdot (\nabla_y w_{2i})\} = 0, & y \in E \\ \sum_{i=1}^3 \{a_{21}(x) \nabla_y \cdot (\nabla_y w_{1i}) + a_{22}(x) \nabla_y \cdot (\nabla_y w_{2i})\} = 0, & y \in E \end{cases}$$

Since the latter equality must be satisfied for each  $x \in \Omega$  it follows that each term must be equal to zero, i.e.

$$\begin{cases} \nabla_y \cdot (\nabla_y w_{1i}) = 0, & y \in E \\ \nabla_y \cdot (\nabla_y w_{2i}) = 0, & y \in E \end{cases}$$

and from here (as well as from the interface conditions) it follows that  $w_{1i}(y) \equiv w_{2i}(y)$  for each  $i = 1, 2, 3$ .

For the functions  $c_1^e$  and  $\phi_1^e$  we have the following interface conditions:

$$\begin{aligned} (k_{11} \nabla_y c_1^e + k_{12} \nabla_y \phi_1^e) \cdot \mathbf{n}_s &= -(k_{11} \nabla_x c_0^e + k_{12} \nabla_x \phi_0^e) \cdot \mathbf{n}_s, & y \in \Gamma \\ (k_{21} \nabla_y c_1^e + k_{22} \nabla_y \phi_1^e) \cdot \mathbf{n}_s &= -(k_{21} \nabla_x c_0^e + k_{22} \nabla_x \phi_0^e) \cdot \mathbf{n}_s, & y \in \Gamma \end{aligned}$$

which according to our notation is equivalent to

$$(K \nabla_y U_1) \cdot \mathbf{n}_s = -(K \nabla_x U_0) \cdot \mathbf{n}_s$$



For  $y \in E$  we have the following system of PDEs and corresponding interface conditions:

$$\begin{aligned} \sum_{i=1}^3 \nabla_y \cdot (K^e V_i) &= 0, \quad y \in E \\ \sum_{i=1}^3 (K^e V_i) \cdot \mathbf{n}_s &= -(K^e \nabla_x U_0) \cdot \mathbf{n}_s, \quad y \in \Gamma \end{aligned}$$

where

$$V_i = C_i \begin{pmatrix} \nabla_y w_{1i} \\ \nabla_y w_{2i} \end{pmatrix}$$

$$K^e(x) C_i(x) = \begin{pmatrix} k_{11}^e & k_{12}^e \\ k_{21}^e & k_{22}^e \end{pmatrix} \begin{pmatrix} \frac{\partial c_0^e}{\partial x_i} & 0 \\ 0 & \frac{\partial \phi_0^e}{\partial x_i} \end{pmatrix} = \begin{pmatrix} k_{11}^e \frac{\partial c_0^e}{\partial x_i} & k_{12}^e \frac{\partial \phi_0^e}{\partial x_i} \\ k_{21}^e \frac{\partial c_0^e}{\partial x_i} & k_{22}^e \frac{\partial \phi_0^e}{\partial x_i} \end{pmatrix}$$

Therefore for the interface conditions we obtain

$$\sum_{i=1}^3 \left[ \begin{pmatrix} k_{11}^e \frac{\partial c_0^e}{\partial x_i} & k_{12}^e \frac{\partial \phi_0^e}{\partial x_i} \\ k_{21}^e \frac{\partial c_0^e}{\partial x_i} & k_{22}^e \frac{\partial \phi_0^e}{\partial x_i} \end{pmatrix} \begin{pmatrix} \nabla_y w_{1i} \\ \nabla_y w_{2i} \end{pmatrix} \right] \cdot \mathbf{n}_s = - \begin{pmatrix} k_{11}^e \nabla_x c_0^e + k_{12}^e \nabla_x \phi_0^e \\ k_{21}^e \nabla_x c_0^e + k_{22}^e \nabla_x \phi_0^e \end{pmatrix} \cdot \mathbf{n}_s$$

which is equivalent to

$$\sum_{i=1}^3 \left[ \begin{pmatrix} k_{11}^e \frac{\partial c_0^e}{\partial x_i} \nabla_y w_{1i} + k_{12}^e \frac{\partial \phi_0^e}{\partial x_i} \nabla_y w_{2i} \\ k_{21}^e \frac{\partial c_0^e}{\partial x_i} \nabla_y w_{1i} + k_{22}^e \frac{\partial \phi_0^e}{\partial x_i} \nabla_y w_{2i} \end{pmatrix} \right] \cdot \mathbf{n}_s = - \begin{pmatrix} k_{11}^e \nabla_x c_0^e + k_{12}^e \nabla_x \phi_0^e \\ k_{21}^e \nabla_x c_0^e + k_{22}^e \nabla_x \phi_0^e \end{pmatrix} \cdot \mathbf{n}_s$$

The latter is equivalent to (according to the previously defined operations)

$$\begin{aligned} \sum_{i=1}^3 \left( k_{11}^e \frac{\partial c_0^e}{\partial x_i} \nabla_y w_{1i} + k_{12}^e \frac{\partial \phi_0^e}{\partial x_i} \nabla_y w_{2i} \right) \cdot \mathbf{n}_s &= - \left( k_{11}^e \sum_{i=1}^3 \frac{\partial c_0^e}{\partial x_i} \mathbf{e}_i + k_{12}^e \sum_{i=1}^3 \frac{\partial \phi_0^e}{\partial x_i} \mathbf{e}_i \right) \cdot \mathbf{n}_s \\ \sum_{i=1}^3 \left( k_{21}^e \frac{\partial c_0^e}{\partial x_i} \nabla_y w_{1i} + k_{22}^e \frac{\partial \phi_0^e}{\partial x_i} \nabla_y w_{2i} \right) \cdot \mathbf{n}_s &= - \left( k_{21}^e \sum_{i=1}^3 \frac{\partial c_0^e}{\partial x_i} \mathbf{e}_i + k_{22}^e \sum_{i=1}^3 \frac{\partial \phi_0^e}{\partial x_i} \mathbf{e}_i \right) \cdot \mathbf{n}_s \end{aligned}$$

which is equivalent to

$$\begin{aligned} \sum_{i=1}^3 \left\{ k_{11}^e(x) \frac{\partial c_0^e}{\partial x_i}(x) (\nabla_y w_{1i} + \mathbf{e}_i) + k_{12}^e(x) \frac{\partial \phi_0^e}{\partial x_i}(x) (\nabla_y w_{2i} + \mathbf{e}_i) \right\} \cdot \mathbf{n}_s &= 0 \\ \sum_{i=1}^3 \left\{ k_{21}^e(x) \frac{\partial c_0^e}{\partial x_i}(x) (\nabla_y w_{1i} + \mathbf{e}_i) + k_{22}^e(x) \frac{\partial \phi_0^e}{\partial x_i}(x) (\nabla_y w_{2i} + \mathbf{e}_i) \right\} \cdot \mathbf{n}_s &= 0 \end{aligned}$$

Since the latter equalities must be satisfied for each  $x \in \Omega$ , it follows that

$$\left| \begin{array}{l} (\nabla_y w_{1i} + \mathbf{e}_i) \cdot \mathbf{n}_s = 0 \\ (\nabla_y w_{2i} + \mathbf{e}_i) \cdot \mathbf{n}_s = 0 \end{array} \right.$$

which is equivalent to

$$\left| \begin{array}{l} \nabla_y w_{1i} \cdot \mathbf{n}_s = -\mathbf{e}_i \cdot \mathbf{n}_s \\ \nabla_y w_{2i} \cdot \mathbf{n}_s = -\mathbf{e}_i \cdot \mathbf{n}_s \end{array} \right.$$

And since we obtained identical PDEs for  $w_{1i}$  and  $w_{2i}$ , for  $i = 1, 2, 3$ , we obtained that  $w_{1i}(y) \equiv w_{2i}(y)$  and the interface conditions are:

$$\nabla_y w_{1i} \cdot \mathbf{n}_s = -\mathbf{e}_i \cdot \mathbf{n}_s, \quad y \in \Gamma \quad (5.79)$$

- After we obtained that  $w_{1i}(y) \equiv w_{2i}(y)$  for  $i = 1, 2, 3$ , we introduce a new notation: we remove the first index "1" from the notation of the function  $w$ .
- Thus we obtain cell problems which turned out to depend only on the geometry of the domain but not on the nonlinear model coefficients  $k_{ij}^e$ .
- Therefore we do not have to solve the cell problems for each  $x \in \Omega$ , but only once for each time step and this will reduce significantly the computational time.
- **Auxiliary Cell Problems:**  $i = 1, 2, 3$

$$\nabla_y \cdot (\nabla_y w_i) = 0, \quad y \in E \quad (5.80a)$$

$$\nabla_y w_i \cdot \mathbf{n}_s = -\mathbf{e}_i \cdot \mathbf{n}_s, \quad y \in \Gamma \quad (5.80b)$$

- Periodic boundary conditions on  $\partial E \setminus \Gamma$ , i.e. on the outer boundary of the electrolyte domain which is not part of the interface
- $\int_E w_i(y) dy = 0, \quad i = 1, 2, 3$  in order to fix the solution

Finally we obtain that

$$c_1^e(x, y, t) = \sum_{i=1}^3 w_i(y, t) \frac{\partial c_0^e}{\partial x_i}(x, t) \quad (5.81)$$

$$\phi_1^e(x, y, t) = \sum_{i=1}^3 w_i(y, t) \frac{\partial \phi_0^e}{\partial x_i}(x, t) \quad (5.82)$$

where  $w_i(y, t)$  and  $\psi_i(y, t)$  are  $Y$ -periodic functions in the  $y$  variable.

### 5.5.2 Order $\varepsilon^0$ : Derivation of the Homogenized Equations

We have the following system of equations for  $y \in Y$  and  $x \in \Omega$

$$\begin{aligned} \chi^e(y) \frac{\partial}{\partial t}(c_0^e) &= \nabla_x \cdot [k_{11}(y, c_0^e) (\nabla_x c_0^e + \nabla_y c_1^e) + k_{12}(y) (\nabla_x \phi_0^e + \nabla_y \phi_1^e)] + \\ &\quad + \nabla_y \cdot [k_{11}(y, c_0^e) \nabla_x c_1^e + k_{11}(y, c_0^e) \nabla_y c_2^e + k_{12}(y) \nabla_x \phi_1^e + k_{12}(y) \nabla_y \phi_2^e] \end{aligned} \quad (5.83a)$$

$$\begin{aligned} &\nabla_x \cdot [k_{21}(y, c_0^e) (\nabla_x c_0^e + \nabla_y c_1^e) + k_{22}(y) (\nabla_x \phi_0^e + \nabla_y \phi_1^e)] + \\ &+ \nabla_y \cdot [k_{21}(y, c_0^e) \nabla_x c_1^e + k_{21}(y, c_0^e) \nabla_y c_2^e + k_{22}(y) \nabla_x \phi_1^e + k_{22}(y) \nabla_y \phi_2^e] = 0 \end{aligned} \quad (5.83b)$$

with periodic boundary conditions on  $\partial Y$  and with the following interface conditions on  $\Gamma$ :

$$- [k_{11}(y, c_0^e) \nabla_x c_1^e + k_{11}(y, c_0^e) \nabla_y c_2^e + k_{12}(y) \nabla_x \phi_1^e + k_{12}(y) \nabla_y \phi_2^e] \cdot \mathbf{n}_s = \frac{1}{\varepsilon} \mathcal{N}(c_0^e, c_0^s, \phi_0^e, \phi_0^s) \quad (5.84a)$$

$$- [k_{21}(y, c_0^e) \nabla_x c_1^e + k_{21}(y, c_0^e) \nabla_y c_2^e + k_{22}(y) \nabla_x \phi_1^e + k_{22}(y) \nabla_y \phi_2^e] \cdot \mathbf{n}_s = \frac{1}{\varepsilon} \mathcal{J}(c_0^e, c_0^s, \phi_0^e, \phi_0^s) \quad (5.84b)$$

Now we integrate both sides of equations (5.83) over the reference periodicity cell  $Y$  and we divide by the measure of  $Y$ , and then we obtain

$$\begin{aligned} \frac{|E|}{|Y|} \frac{\partial c_0^e}{\partial t} &= \frac{1}{|Y|} \int_Y \nabla_x \cdot [k_{11}(y, c_0^e) (\nabla_x c_0^e + \nabla_y c_1^e) + k_{12}(y) (\nabla_x \phi_0^e + \nabla_y \phi_1^e)] dy + \\ &\quad + \frac{1}{|Y|} \int_Y \nabla_y \cdot [k_{11}(y, c_0^e) \nabla_x c_1^e + k_{11}(y, c_0^e) \nabla_y c_2^e + k_{12}(y) \nabla_x \phi_1^e + k_{12}(y) \nabla_y \phi_2^e] dy \end{aligned} \quad (5.85a)$$

$$\begin{aligned} &\frac{1}{|Y|} \int_Y \nabla_x \cdot [k_{21}(y, c_0^e) (\nabla_x c_0^e + \nabla_y c_1^e) + k_{22}(y) (\nabla_x \phi_0^e + \nabla_y \phi_1^e)] dy + \\ &+ \frac{1}{|Y|} \int_Y \nabla_y \cdot [k_{21}(y, c_0^e) \nabla_x c_1^e + k_{21}(y, c_0^e) \nabla_y c_2^e + k_{22}(y) \nabla_x \phi_1^e + k_{22}(y) \nabla_y \phi_2^e] dy = 0 \end{aligned} \quad (5.85b)$$

In equation (5.85a) for the left hand side we have

$$\frac{1}{|Y|} \int_Y \chi^e(y) \frac{\partial c_0^e}{\partial t}(x, t) dy = \frac{1}{|Y|} \frac{\partial c_0^e}{\partial t} \int_Y \chi^e(y) dy = \frac{1}{|Y|} \frac{\partial c_0^e}{\partial t} \left( \int_E 1 dy + \int_S 0 dy \right) = \frac{|E|}{|Y|} \frac{\partial c_0^e}{\partial t} \quad (5.86)$$

Since  $Y = E \cup S$  and

$$k_{ij}(y, c_0^e) = \chi^e(y) k_{ij}^e = \begin{cases} k_{ij}^e, & y \in E \\ 0, & y \in S \end{cases}$$

then it follows that

$$\frac{1}{|Y|} \int_Y k_{ij}(y, c_0^e)(\dots) dy = \frac{1}{|Y|} \left( \int_E k_{ij}^e(\dots) dy + \underbrace{\int_S 0(\dots) dy}_{=0} \right) = \frac{1}{|Y|} \int_E k_{ij}^e(\dots) dy$$

Now we consider the second integral of the right hand side of equation (5.85a):

$$\begin{aligned} & \frac{1}{|Y|} \int_E \nabla_y \cdot [k_{11}^e(c_0^e) \nabla_x c_1^e + k_{11}^e(c_0^e) \nabla_y c_2^e + k_{12}^e \nabla_x \phi_1^e + k_{12}^e \nabla_y \phi_2^e] dy = \\ & = \frac{1}{|Y|} \int_{\partial E} [k_{11}^e(c_0^e) \nabla_x c_1^e + k_{11}^e(c_0^e) \nabla_y c_2^e + k_{12}^e \nabla_x \phi_1^e + (k_{12}^e)_0 \nabla_y \phi_2^e] \cdot \mathbf{n} ds = \\ & = \frac{1}{|Y|} \int_{\partial E \cap \partial Y} \underbrace{[k_{11}^e(c_0^e) \nabla_x c_1^e + k_{11}^e(c_0^e) \nabla_y c_2^e + k_{12}^e \nabla_x \phi_1^e + k_{12}^e \nabla_y \phi_2^e] \cdot \mathbf{n}}_{=0} ds + \\ & + \frac{1}{|Y|} \int_{\Gamma} [k_{11}^e(c_0^e) \nabla_x c_1^e + k_{11}^e(c_0^e) \nabla_y c_2^e + k_{12}^e \nabla_x \phi_1^e + k_{12}^e \nabla_y \phi_2^e] \cdot \mathbf{n}_e ds = \\ & = 0 - \frac{1}{|Y|} \int_{\Gamma} [k_{11}^e(c_0^e) \nabla_x c_1^e + k_{11}^e(c_0^e) \nabla_y c_2^e + k_{12}^e \nabla_x \phi_1^e + k_{12}^e \nabla_y \phi_2^e] \cdot \mathbf{n}_s ds = \\ & = \frac{1}{\varepsilon |Y|} \int_{\Gamma} \mathcal{N}(c_0^e, c_0^s, \phi_0^e, \phi_0^s) ds \end{aligned}$$

For the first integral in the right hand side of equation (5.85a) we obtain:

$$\begin{aligned} & \frac{1}{|Y|} \int_E \nabla_x \cdot [k_{11}^e \nabla_y c_1^e + k_{12}^e \nabla_y \phi_1^e + k_{11}^e \nabla_x c_0^e + k_{12}^e \nabla_x \phi_0^e] dy = \\ & = \frac{1}{|Y|} \int_E \nabla_x \cdot \left[ k_{11}^e \sum_{i=1}^3 \frac{\partial c_0^e}{\partial x_i} \nabla_y w_i + k_{12}^e \sum_{i=1}^3 \frac{\partial \phi_0^e}{\partial x_i} \nabla_y w_i + k_{11}^e \nabla_x c_0^e + k_{12}^e \nabla_x \phi_0^e \right] dy = \\ & = \nabla_x \cdot \left\{ \frac{1}{|Y|} \int_E \left[ k_{11}^e \sum_{i=1}^3 \frac{\partial c_0^e}{\partial x_i} \nabla_y w_i + k_{12}^e \sum_{i=1}^3 \frac{\partial \phi_0^e}{\partial x_i} \nabla_y w_i + k_{11}^e \nabla_x c_0^e + k_{12}^e \nabla_x \phi_0^e \right] dy \right\} = \\ & = \nabla_x \cdot \left\{ \sum_{i=1}^3 \frac{1}{|Y|} \int_E k_{11}^e \frac{\partial c_0^e}{\partial x_i}(x) \nabla_y w_i dy + \sum_{i=1}^3 \frac{1}{|Y|} \int_E k_{12}^e \frac{\partial \phi_0^e}{\partial x_i}(x) \nabla_y w_i dy + \right. \\ & \quad \left. + \frac{1}{|Y|} \int_E k_{11}^e \nabla_x c_0^e dy + \frac{1}{|Y|} \int_E k_{12}^e \nabla_x \phi_0^e dy \right\} = \end{aligned}$$

$$\begin{aligned}
&= \nabla_x \cdot \left\{ \sum_{i=1}^3 \left( \frac{1}{|Y|} \int_E k_{11}^e \nabla_y w_i dy \right) \frac{\partial c_0^e}{\partial x_i}(x) + \sum_{i=1}^3 \left( \frac{1}{|Y|} \int_E k_{12}^e \nabla_y w_i dy \right) \frac{\partial \phi_0^e}{\partial x_i}(x) + \right. \\
&\quad \left. + \left( \frac{1}{|Y|} \int_E k_{11}^e dy \right) \nabla_x c_0^e + \left( \frac{1}{|Y|} \int_E k_{12}^e dy \right) \nabla_x \phi_0^e \right\} = \\
&= \nabla_x \cdot \left\{ A \nabla_x c_0^e + B \nabla_x \phi_0^e + k_{11}^e \frac{|E|}{|Y|} I \nabla_x c_0^e + k_{12}^e \frac{|E|}{|Y|} I \nabla_x \phi_0^e \right\} = \\
&= \nabla_x \cdot \left\{ \left( A + k_{11}^e \frac{|E|}{|Y|} I \right) \nabla_x c_0^e + \left( B + k_{12}^e \frac{|E|}{|Y|} I \right) \nabla_x \phi_0^e \right\}
\end{aligned}$$

where  $I$  is the identity matrix and

$$\begin{aligned}
A &= (a_{ij})_{i,j=1}^3 = \frac{1}{|Y|} \int_E k_{11}^e \frac{\partial w_j}{\partial y_i}(y) dy \\
B &= (b_{ij})_{i,j=1}^3 = \frac{1}{|Y|} \int_E k_{12}^e \frac{\partial w_j}{\partial y_i}(y) dy
\end{aligned}$$

Now we denote

$$\begin{aligned}
\mathbf{K}_{11} &= A + k_{11}^e \frac{|E|}{|Y|} I \\
\mathbf{K}_{12} &= B + k_{12}^e \frac{|E|}{|Y|} I
\end{aligned}$$

Then

$$\begin{aligned}
(\mathbf{K}_{11})_{ij} &= \frac{1}{|Y|} \int_E k_{11}^e \frac{\partial w_j}{\partial y_i}(y) dy + k_{11}^e \frac{|E|}{|Y|} \delta_{ij} = \\
&= \frac{k_{11}^e}{|Y|} \int_E \left( \delta_{ij} + \frac{\partial w_j}{\partial y_i}(y) \right) dy \tag{5.87}
\end{aligned}$$

We obtain the following homogenized equations:

$$\frac{|E|}{|Y|} \frac{\partial c_0^e}{\partial t} - \nabla_x \cdot (\mathbf{K}_{11} \nabla_x c_0^e + \mathbf{K}_{12} \nabla_x \phi_0^e) = \frac{1}{\varepsilon |Y|} \int_{\Gamma} \mathcal{N}(c_0^e, c_0^s, \phi_0^e, \phi_0^s) ds \tag{5.88}$$

$$-\nabla_x \cdot (\mathbf{K}_{21} \nabla_x c_0^e + \mathbf{K}_{22} \nabla_x \phi_0^e) = \frac{1}{\varepsilon |Y|} \int_{\Gamma} \mathcal{J}(c_0^e, c_0^s, \phi_0^e, \phi_0^s) ds \tag{5.89}$$

where  $\Gamma$  is the interface boundary between the electrolyte and the solid in a single representative periodicity cell  $Y = E \cup S$  and the matrices  $\mathbf{K}_{11}$ ,  $\mathbf{K}_{12}$ ,  $\mathbf{K}_{21}$  and  $\mathbf{K}_{22}$  are

given by:

$$(\mathbf{K}_{11})_{ij} = \frac{k_{11}^e(c_0^e)}{|Y|} \int_E \left( \delta_{ij} + \frac{\partial w_j}{\partial y_i}(y) \right) dy, \quad (\mathbf{K}_{12})_{ij} = \frac{k_{12}^e}{|Y|} \int_E \left( \delta_{ij} + \frac{\partial w_j}{\partial y_i}(y) \right) dy$$

$$(\mathbf{K}_{21})_{ij} = \frac{k_{21}^e(c_0^e)}{|Y|} \int_E \left( \delta_{ij} + \frac{\partial w_j}{\partial y_i}(y) \right) dy, \quad (\mathbf{K}_{22})_{ij} = \frac{k_{22}^e}{|Y|} \int_E \left( \delta_{ij} + \frac{\partial w_j}{\partial y_i}(y) \right) dy$$

## 5.6 Homogenization of the Solid Phase PDEs

We will homogenize only the governing equation for the potential  $\phi_\varepsilon^s(x)$ .

From  $\mathbf{J}_\varepsilon^s \cdot \mathbf{n}_s = \mathcal{J}_\varepsilon$  for the interface conditions we obtain:

$$\varepsilon^{-2} : \quad 0 = \kappa(y) \nabla_y \phi_0^s \cdot \mathbf{n}_s \quad (5.90a)$$

$$\varepsilon^{-1} : \quad 0 = \kappa(y) (\nabla_x \phi_0^s + \nabla_y \phi_1^s) \cdot \mathbf{n}_s \quad (5.90b)$$

$$\varepsilon^0 : \quad \frac{1}{\varepsilon} \mathcal{J}(c_0^e, c^s, \phi_0^e, \phi_0^s) = \quad (5.90c)$$

$$= -(\kappa(y) \nabla_x \phi_1^s + \kappa(y) \nabla_y \phi_2^s) \cdot \mathbf{n}_s \quad (5.90d)$$

### 5.6.1 Homogenization of the PDEs: Order $\varepsilon^{-2}$

We have the equation

$$\nabla_y \cdot (\kappa(y) \nabla_y \phi_0^s(x, y, t)) = 0, \quad y \in Y \quad (5.91)$$

which is equivalent to

$$\nabla_y \cdot (\kappa^s \nabla_y \phi_0^s(x, y, t)) = 0, \quad y \in S \quad (5.92)$$

with the following interface conditions:

$$\kappa^s \nabla_y \phi_0^s \cdot \mathbf{n}_s = 0, \quad y \in \Gamma \equiv \partial S \quad (5.93)$$

From here (and taking into account the boundary conditions), we obtain that

$$\phi_0^s = \phi_0^s(x, t) \quad (5.94)$$

which coincides with the assumption we made that  $\phi_0^s$  is a function of  $x$  only.

### 5.6.2 Homogenization of the PDEs: Order $\varepsilon^{-1}$

We have the following equation for  $y \in Y$ :

$$\nabla_x \cdot (\kappa(y) \nabla_y \phi_0^s(x, t)) + \nabla_y \cdot (\kappa(y) \nabla_x \phi_0^s(x, t) + \kappa(y) \nabla_y \phi_1^s(x, y, t)) = 0 \quad (5.95)$$

with periodic boundary conditions on  $\partial Y$  for the  $Y$ -periodic functions  $c_1^s(x, y, t)$  and  $\phi_1^s(x, y, t)$ , and the following interface conditions on  $\Gamma \equiv \partial S$ :

$$(\kappa(y) \nabla_x \phi_0^s + \kappa(y) \nabla_y \phi_1^s) \cdot \mathbf{n}_s = 0, \quad y \in \Gamma \quad (5.96)$$

Since  $\nabla_y \phi_0^s = 0$  because  $\phi_0^s = \phi_0^s(x, t)$ , the latter equation becomes

$$\nabla_y \cdot (\kappa(y) \nabla_x \phi_0^s(x, t) + \kappa(y) \nabla_y \phi_1^s(x, y, t)) = 0, \quad y \in Y \quad (5.97)$$

We look for the solution  $\phi_1^s$  of equation (5.97) (provided that we consider the function  $\phi_0^s$  given) in the following form

$$\phi_1^s(x, y, t) = \sum_{i=1}^3 \varphi_i^s(y) \frac{\partial \phi_0^s}{\partial x_i}(x, t) \quad (5.98)$$

where the  $Y$ -periodic function  $\varphi_l^s(y)$  for  $l = 1, 2, 3$  in  $3D$  is the solution of the following auxiliary cell problem for  $l = 1, 2, 3$ :

- ”Solid” Cell Problem for  $l = 1, 2, 3$ :

–

$$\nabla \cdot (\nabla_y \varphi_l^s) = 0, \quad y \in S \quad (5.99a)$$

$$\nabla_y \varphi_l^s \cdot \mathbf{n}_s = -\mathbf{e}_l \cdot \mathbf{n}_s, \quad y \in \Gamma \quad (5.99b)$$

– Periodic boundary conditions on  $\partial S \setminus \Gamma$ , i.e. on the boundary of the particles where the particles are connected

$$- \int_S \varphi_l^s(y) dy = 0, \quad l = 1, 2, 3 \text{ in order to fix the solution}$$

### 5.6.3 Homogenization of the PDEs: Order $\varepsilon^0$

He have the following equation for  $y \in Y$ :

$$\nabla_x \cdot (\kappa(y) \nabla_x \phi_0^s + \kappa(y) \nabla_y \phi_1^s) + \nabla_y \cdot (\kappa(y) \nabla_x \phi_1^s + \kappa(y) \nabla_y \phi_2^s) = 0 \quad (5.100)$$

with periodic boundary conditions on  $\partial Y$  and the following interface conditions on  $\Gamma \equiv \partial S$ :

$$-(\kappa(y) \nabla_x \phi_1^s + \kappa(y) \nabla_y \phi_2^s) \cdot \mathbf{n}_s = \frac{1}{\varepsilon} \mathcal{J}(c_0^e, c_0^s, \phi_0^e, \phi_0^s), \quad y \in \Gamma = \partial S \quad (5.101)$$

After we integrate the equation over  $Y$  and after we substitute  $\phi_1^s(x, y, t)$  with its equal expression from (5.98), we obtain the homogenized equation:

$$-\nabla_x \cdot (\Lambda^s \nabla_x \phi_0^s) = -\frac{1}{\varepsilon |Y|} \int_{\Gamma} \mathcal{J}(c_0^e, c_0^s, \phi_0^e, \phi_0^s) ds \quad (5.102)$$

where

$$(\Lambda^s)_{ij} = \frac{1}{|Y|} \int_S \kappa^s \left( \delta_{ij} + \frac{\partial \varphi_j^s}{\partial y_i} \right) dy \quad (5.103)$$

## 5.7 Homogenized Problem Without Boundary Conditions

Macroscale equations:

$$\frac{|E|}{|Y|} \frac{\partial c_0^e}{\partial t} - \nabla_x \cdot (\mathbf{K}_{11} \nabla_x c_0^e + \mathbf{K}_{12} \nabla_x \phi_0^e) = \frac{1}{\varepsilon |Y|} \int_{\Gamma} \mathcal{N}(c_0^e, c^s, \phi_0^e, \phi_0^s) ds, \quad x \in \Omega \quad (5.104a)$$

$$-\nabla_x \cdot (\mathbf{K}_{21} \nabla_x c_0^e + \mathbf{K}_{22} \nabla_x \phi_0^e) = \frac{1}{\varepsilon |Y|} \int_{\Gamma} \mathcal{J}(c_0^e, c^s, \phi_0^e, \phi_0^s) ds, \quad x \in \Omega \quad (5.104b)$$

$$-\nabla_x \cdot (\Lambda^s \nabla_x \phi_0^s) = -\frac{1}{\varepsilon |Y|} \int_{\Gamma} \mathcal{J}(c_0^e, c^s, \phi_0^e, \phi_0^s) ds, \quad x \in \Omega \quad (5.104c)$$

Microscale equation:

$$\frac{\partial c^s}{\partial t} - \nabla_y \cdot \left( \frac{D^s}{\varepsilon^2} \nabla_y c^s \right) = 0, \quad y \in S \quad (5.105a)$$

$$-\frac{D^s}{\varepsilon^2} \nabla_y c^s \cdot \mathbf{n}_s = \frac{1}{\varepsilon} \mathcal{N}(c_0^e, c^s, \phi_0^e, \phi_0^s), \quad y \in \Gamma \quad (5.105b)$$

## 6 Homogenization of the Neumann Boundary Conditions

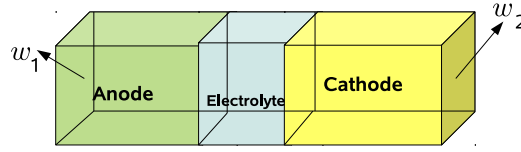


Figure 19: Battery Cell

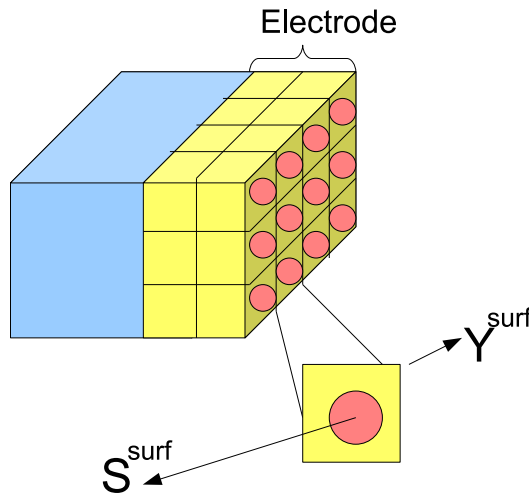


Figure 20: Electrode Outer Boundary



We have the following Neumann boundary condition in the  $\varepsilon$ -setting of the original microscopic problem:

$$-\kappa_\varepsilon \nabla \phi_\varepsilon^s \cdot \mathbf{n} = E_2^\varepsilon, \quad x \in \omega_2 \quad (6.1)$$

where

- $E_2^\varepsilon = \chi_\varepsilon^s(x) E_2^s = \chi^s\left(\frac{x}{\varepsilon}\right) E_2^s = \chi^s(y) E_2^s$
- $\kappa_\varepsilon(x) = \kappa\left(\frac{x}{\varepsilon}\right) = \chi^s\left(\frac{x}{\varepsilon}\right) \kappa^s = \chi^s(y) \kappa^s$
- $\nabla = \nabla_x + \frac{1}{\varepsilon} \nabla_y$
- $\phi_\varepsilon^s(x) = \phi_0^s(x) + \varepsilon \phi_1^s(x, y) + \varepsilon^2 \phi_2^s(x, y)$  and therefore
- $\nabla \phi_\varepsilon^s = \nabla_x \phi_0^s + \nabla_y \phi_1^s + O(\varepsilon) \xrightarrow{\varepsilon \rightarrow 0} \nabla_x \phi_0^s + \nabla_y \phi_1^s$
- $\phi_1^s(x, y) = \sum_{i=1}^3 \varphi_i^s(y) \frac{\partial \phi_0^s}{\partial x_i}(x)$

Let  $\mathbf{n} = (n_1, n_2, n_3)$ . Now we calculate the flux

$$\begin{aligned} \kappa_\varepsilon \nabla \phi_\varepsilon^s \cdot \mathbf{n} &= \kappa(y) (\nabla_x \phi_0^s + \nabla_y \phi_1^s) \cdot \mathbf{n} = \\ &= \kappa(y) \left( \frac{\partial \phi_0^s}{\partial x_1} n_1 + \frac{\partial \phi_1^s}{\partial y_1} n_1 + \frac{\partial \phi_0^s}{\partial x_2} n_2 + \frac{\partial \phi_1^s}{\partial y_2} n_2 \right) = \\ &= \kappa(y) \left( \frac{\partial \phi_0^s}{\partial x_1} n_1 + \frac{\partial \varphi_1^s}{\partial y_1} \frac{\partial \phi_0^s}{\partial x_1} n_1 + \frac{\partial \varphi_2^s}{\partial y_1} \frac{\partial \phi_0^s}{\partial x_2} n_1 + \right. \\ &\quad \left. + \frac{\partial \phi_0^s}{\partial x_2} n_2 + \frac{\partial \varphi_1^s}{\partial y_2} \frac{\partial \phi_0^s}{\partial x_1} n_2 + \frac{\partial \varphi_2^s}{\partial y_2} \frac{\partial \phi_0^s}{\partial x_2} n_2 \right) = \\ &= \frac{\partial \phi_0^s}{\partial x_1} \left( \kappa(y) \left( 1 + \frac{\partial \varphi_1^s}{\partial y_1} \right) \right) n_1 + \kappa(y) \frac{\partial \phi_0^s}{\partial x_2} \frac{\partial \varphi_2^s}{\partial y_1} n_1 + \\ &+ \frac{\partial \phi_0^s}{\partial x_2} \left( \kappa(y) \left( 1 + \frac{\partial \varphi_2^s}{\partial y_2} \right) \right) n_2 + \kappa(y) \frac{\partial \phi_0^s}{\partial x_1} \frac{\partial \varphi_1^s}{\partial y_2} n_2 = \\ &= \frac{\partial \phi_0^s}{\partial x_1} A_{11} n_1 + \frac{\partial \phi_0^s}{\partial x_2} A_{12} n_1 + \frac{\partial \phi_0^s}{\partial x_2} A_{22} n_2 + \frac{\partial \phi_0^s}{\partial x_1} A_{21} n_2 = \\ &= \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} \begin{pmatrix} \frac{\partial \phi_0^s}{\partial x_1} \\ \frac{\partial \phi_0^s}{\partial x_2} \end{pmatrix} \cdot \mathbf{n} = (A \nabla_x \phi_0^s) \cdot \mathbf{n} \end{aligned} \quad (6.2)$$

where we denote  $A_{ij} = \kappa(y) \left( \delta_{ij} + \frac{\partial \varphi_j^s}{\partial y_i} \right) = \chi^s(y) \kappa^s \left( \delta_{ij} + \frac{\partial \varphi_j^s}{\partial y_i}(y) \right)$ . Therefore we obtain

$$-(A \nabla_x \phi_0^s) \cdot \mathbf{n} = \chi^s(y) E_2^s, \quad x \in \omega_2 \quad (y \in Y^{surf}) \quad (6.3)$$

Now we integrate over  $S$  (in order to obtain the coefficients  $\Lambda^s$  and respectively the flux  $\Lambda^s \nabla \phi_0^s$ , see Figure 20 ) both sides of equality (6.3) and we obtain

$$-\frac{1}{|Y^{surf}|} \int_{S^{surf}} (A \nabla_x \phi_0^s) \cdot \mathbf{n} dS = \frac{1}{|Y^{surf}|} \int_{S^{surf}} \chi^s(y) E_2^s dS, \quad x \in \omega_2 \quad (6.4)$$

which is equivalent to

$$\begin{aligned}
- (\Lambda^s \nabla_x \phi_0^s) \cdot \mathbf{n} &= \frac{1}{|Y^{surf}|} \int_{S^{surf}} 1 E_2^s dS, \quad x \in \omega_2 \iff \\
- (\Lambda^s \nabla_x \phi_0^s) \cdot \mathbf{n} &= \frac{E_2^s}{|Y^{surf}|} \int_{S^{surf}} 1 dS, \quad x \in \omega_2 \iff \\
- (\Lambda^s \nabla_x \phi_0^s) \cdot \mathbf{n} &= \frac{|S^{surf}|}{|Y^{surf}|} E_2^s, \quad x \in \omega_2
\end{aligned} \tag{6.5}$$

### Upscaled Neumann BC: Verification

We denote the flux

$$- \Lambda^s \nabla \phi_0^s \cdot \mathbf{n} = C = const \tag{6.6}$$

Let us also denote with  $p = p(\varepsilon)$  the number of all periodicity cells which have an outer boundary on the external cathode (electrode) boundary  $\omega_2$  (for simplicity we fix  $\omega_2$  to be the external cathode boundary, i.e.  $\omega_2$  consists of both solid particles and electrolyte, whereas with  $\partial\Omega_c$  we denote only the cathode solid particles outer boundary). Since the total flux across  $\omega_2$  should be preserved, i.e. it must be the same in both the upscaled problem and the initial microscopic one, we want to ensure that the following surface integrals are equal

$$\int_{\omega_2 \cap \partial\Omega_c} -\kappa_\varepsilon(x) \nabla \phi_\varepsilon^s \cdot \mathbf{n} dS = \int_{\omega_2} -\Lambda^s \nabla \phi_0^s \cdot \mathbf{n} dS$$

which is equivalent to

$$\begin{aligned}
\int_{\omega_2 \cap \partial\Omega_c} E_2^\varepsilon dS &= \int_{\omega_2} C dS \iff \\
\int_{\omega_2 \cap \partial\Omega_c} \chi_\varepsilon^s(x) E_2^s dS &= \int_{\omega_2} C dS \iff \\
\int_{\omega_2 \cap \partial\Omega_c} E_2^s dS &= \int_{\omega_2} C dS \iff \\
E_2^s \int_{\omega_2 \cap \partial\Omega_c} 1 dS &= C \int_{\omega_2} 1 dS \iff
\end{aligned}$$

$$E_2^s |\omega_2 \cap \partial\Omega_c| = C |\omega_2| \iff$$

$$E_2^s p(\varepsilon) |S^{surf}| = C p(\varepsilon) |Y^{surf}| \iff$$

$$p(\varepsilon) (E_2^s |S^{surf}| - C |Y^{surf}|) = 0 \iff$$

$$E_2^s |S^{surf}| - C |Y^{surf}| = 0 \quad (p(\varepsilon) \neq 0) \iff$$

$$C = \frac{|S^{surf}|}{|Y^{surf}|} E_2^s$$

which is true (we obtained the same result via the homogenization method).

## 7 Homogenized Problem

### 7.1 Macroscale Problem

We obtain the following homogenized equations for the concentration  $c^e$  of ions in the electrolyte, the potential  $\phi^e$  in the electrolyte and for the potential  $\phi^s$  in the solid

$$\frac{|E|}{|Y|} \frac{\partial c_0^e}{\partial t} - \nabla_x \cdot (\mathbf{K}_{11} \nabla_x c_0^e + \mathbf{K}_{12} \nabla_x \phi_0^e) = \frac{1}{\varepsilon |Y|} \int_{\Gamma} \mathcal{N}(c_0^e, c^s, \phi_0^e, \phi_0^s) ds, \quad x \in \Omega \quad (7.1a)$$

$$-\nabla_x \cdot (\mathbf{K}_{21} \nabla_x c_0^e + \mathbf{K}_{22} \nabla_x \phi_0^e) = \frac{1}{\varepsilon |Y|} \int_{\Gamma} \mathcal{J}(c_0^e, c^s, \phi_0^e, \phi_0^s) ds, \quad x \in \Omega \quad (7.1b)$$

$$-\nabla_x \cdot (\Lambda^s \nabla_x \phi_0^s) = -\frac{1}{\varepsilon |Y|} \int_{\Gamma} \mathcal{J}(c_0^e, c^s, \phi_0^e, \phi_0^s) ds, \quad x \in \Omega \quad (7.1c)$$

with the following boundary conditions

$$\phi_0^s = E_1^s, \quad x \in \omega_1 \quad (7.2a)$$

$$(\Lambda^s \nabla_x \phi_0^s) \cdot \mathbf{n} = \frac{|S^{surf}|}{|Y^{surf}|} E_2^s, \quad x \in \omega_2 \quad (7.2b)$$

$$\mathbf{N}_e^h \cdot \mathbf{n} = \mathbf{N}_s^h \cdot \mathbf{n} = 0, \quad x \in \partial\Omega \quad (7.2c)$$

$$\mathbf{J}_e^h \cdot \mathbf{n} = \mathbf{J}_s^h \cdot \mathbf{n} = 0, \quad x \in \partial\Omega \quad (7.2d)$$

and homogenized coefficients (which are tensors)

$$\begin{aligned} (\mathbf{K}_{11})_{ij} &= \frac{k_{11}^e(c_0^e)}{|Y|} \int_E \left( \delta_{ij} + \frac{\partial w_j}{\partial y_i}(y) \right) dy, & (\mathbf{K}_{12})_{ij} &= \frac{k_{12}^e}{|Y|} \int_E \left( \delta_{ij} + \frac{\partial w_j}{\partial y_i}(y) \right) dy \\ (\mathbf{K}_{21})_{ij} &= \frac{k_{21}^e(c_0^e)}{|Y|} \int_E \left( \delta_{ij} + \frac{\partial w_j}{\partial y_i}(y) \right) dy, & (\mathbf{K}_{22})_{ij} &= \frac{k_{22}^e}{|Y|} \int_E \left( \delta_{ij} + \frac{\partial w_j}{\partial y_i}(y) \right) dy \end{aligned} \quad (7.3)$$

$$(\Lambda^s)_{ij} = \frac{1}{|Y|} \int_S \kappa^s \left( \delta_{ij} + \frac{\partial \varphi_j^s}{\partial y_i} \right) dy$$

with  $w_j(y)$  and  $\varphi_j^s(y)$  ( $j = 1, 2, 3$ ) being the solutions of the auxiliary cell problems (5.80a)-(5.80b) and (5.99a)-(5.99b), respectively.

### 7.2 Microscale Problem

We have to solve the following microscale problem for the concentration of ions in the active particles

$$\frac{\partial c^s}{\partial t} - \nabla_y \cdot \left( \frac{D^s}{\varepsilon^2} \nabla_y c^s \right) = 0, \quad y \in S \quad (7.4a)$$

$$-\frac{D^s}{\varepsilon^2} \nabla_y c^s \cdot \mathbf{n}_s = \frac{1}{\varepsilon} \mathcal{N}(c_0^e, c^s, \phi_0^e, \phi_0^s), \quad y \in \Gamma \quad (7.4b)$$

We impose periodic boundary conditions on  $\partial S \setminus \Gamma$ , i.e. on the boundary of the solid particle where the particles are connected to each other.

## 8 Numerical Methods

Since the processes in the homogenized equations are essentially one-dimensional, we can solve them in 1D but we leave the microscale problem for  $c^s$  in 3D. For the space discretization we use the Finite Element Method with linear Lagrange elements. For the time discretization we apply the Backward Euler Method and for the linearization of the resulting system of algebraic equations we use the Newton Method.

For each node in the space discretization of the 1D problem we assume to have one active particle. Therefore we solve as many microscale problems as there are nodes in the discretization of equations (7.1).

We use the following time-stepping scheme. First we solve the homogenized equations (7.1) using Backward Euler Method and using the values of  $c^s$  from the previous time step. Then we use the obtained values  $c^e$ ,  $\phi^e$  and  $\phi^s$  to solve the microscale problem for  $c^s$ .

## 9 Numerical Results

In all the numerical experiments we consider a battery cell which consists of two electrodes— anode and cathode, each of them being a cube with length of the side  $100 \mu\text{m}$  (see Figure 21). Between the two electrodes there is a layer of pure electrolyte with thickness of  $10 \mu\text{m}$ . In each of the experiments we run simulations varying the size of the active particles. We begin with particles having a characteristic size of  $20 \mu\text{m}$  and we decrease this size up to  $2.5 \mu\text{m}$  in the last experiment. In Table 1 we give the values of all the parameters which we use for our computations.

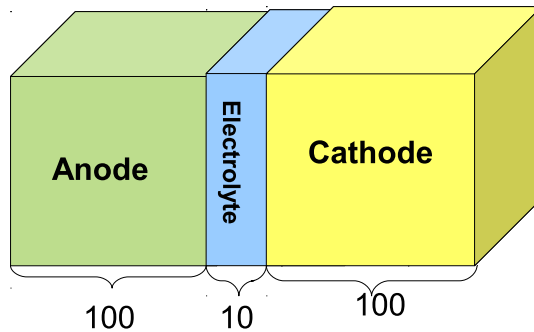


Figure 21: Battery Cell Dimensions

Table 1: Values of the parameters used for the simulations

	$D$	$t_+$	$\kappa$	$c_{max}$	$c_{initial}$	$k$ -reaction rate
Electrolyte	$7.5 \times 10^{-7}$	0.363	0.002	-	0.001	-
Cathode	$1.0 \times 10^{-9}$	0	0.038	0.023671	$0.9 * c_{max}$	0.2
Anode	$3.9 \times 10^{-10}$	0	1.0	0.024681	$0.1 * c_{max}$	0.002

For the open circuit potential  $U_0$  we have

$$U_0(c^s) = -0.132 + 1.41e^{-3.52soc}, \quad x \in \Omega_a \quad (9.1a)$$

$$U_0(c^s) = 4.06279 + 0.0677504 \tanh(-21.8502soc + 12.8268) - 0.045e^{-71.69soc^8} - 0.105734 \left( \frac{1}{(1.00167 - soc)^{0.379571}} - 1.576 \right) + 0.01e^{-200(soc-0.19)}, \quad x \in \Omega_c \quad (9.1b)$$

where

$$soc = \frac{c^s}{c_{max}^s} \quad (9.2)$$

The applied current on the cathode is:

$$(\Lambda^s \nabla_x \phi_0^s) \cdot \mathbf{n} = \frac{|S_{surf}|}{|Y_{surf}|} E_2^s, \quad x \in \omega_2, \quad (9.3)$$

$$E_2^s = 0.01 \quad (9.4)$$

For the potential  $\phi^s$  on the anode outer boundary we impose the following values:

$$\phi_0^s = E_1^s = U_0(c_{initial}^s) = 0.8596, \quad x \in \omega_1 \quad (9.5)$$

We run all the simulations with time step of 2s and with  $t$  we denote the number of time steps.

## 9.1 Experiment 1

We run simulations for 5 active particles in each direction, which means that we have a total number of 125 particles in each electrode. The characteristic size of the particles in this case is  $l = 20 \mu\text{m}$ , whereas the size of the whole electrode is  $L = 100 \mu\text{m}$ . Consequently  $\varepsilon = \frac{l}{L} = 0.2$  in this simulation. In Figure 22 and Figure 23 we compare the results from the full microscopic simulation and the homogenized problem. In all the subsequent numerical experiments we show the results for the potential  $\phi^s$  only in the cathode, since throughout the simulation the values of the potential in the anode are virtually constant. The potential  $\phi^e$  in the electrolyte after 40 time steps is shown in Figure 22. In Figure 23 we show the concentration  $c^s$  in the second layer anode active particle in both the homogenized model and the microscale model. As we can see from the picture, the values of the concentration in both models are pretty close.

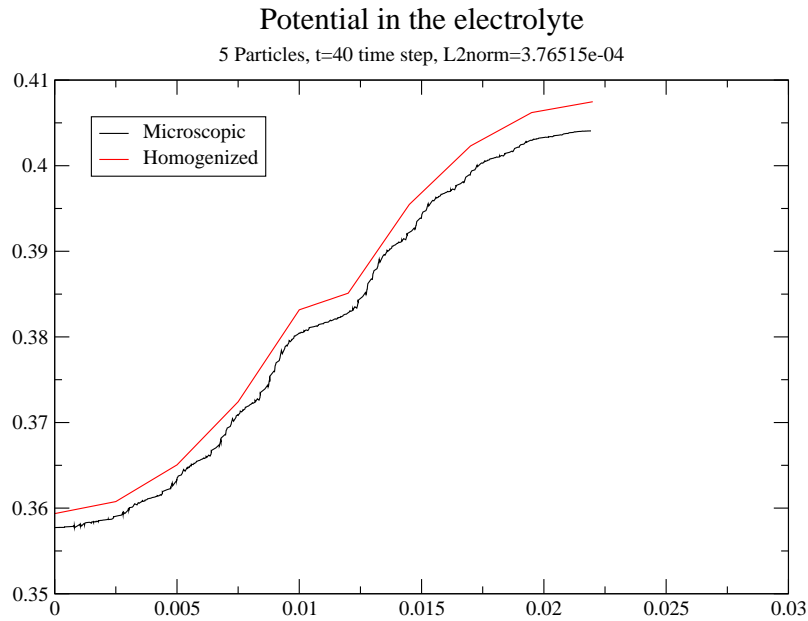


Figure 22: Comparison between the homogenized and the microscopic solution: potential in the electrolyte for  $5 \times 5 \times 5$  particles in each electrode

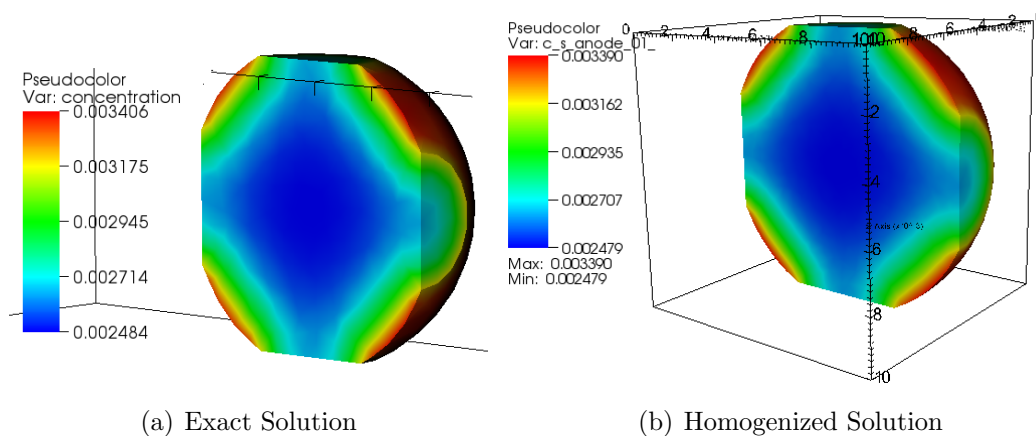


Figure 23: Concentration in the Anode after 80 time steps for 125 particles in each electrode

## 9.2 Experiment 2

We run simulations for 10 active particles in each direction, which means that we have a total number of 1000 particles in each electrode. Therefore the characteristic size of each particle is  $10 \mu\text{m}$  and  $\varepsilon = 0.1$ . The results from the full microscopic simulation and from the homogenized problem are shown in Figure 24, 25, 26 and 27.

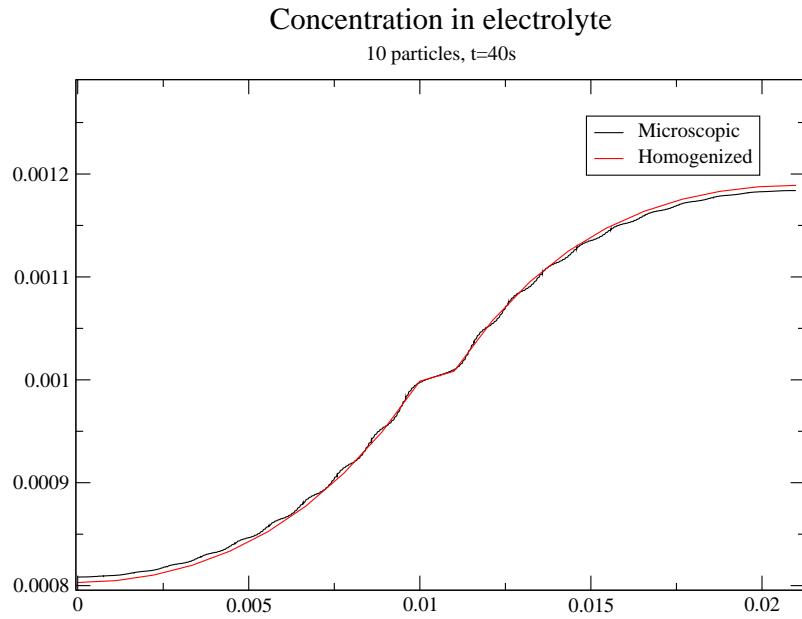


Figure 24: Comparison between the homogenized and the microscopic solution: concentration of  $\text{Li}^+$  in the electrolyte for  $10 \times 10 \times 10$  particles in each electrode

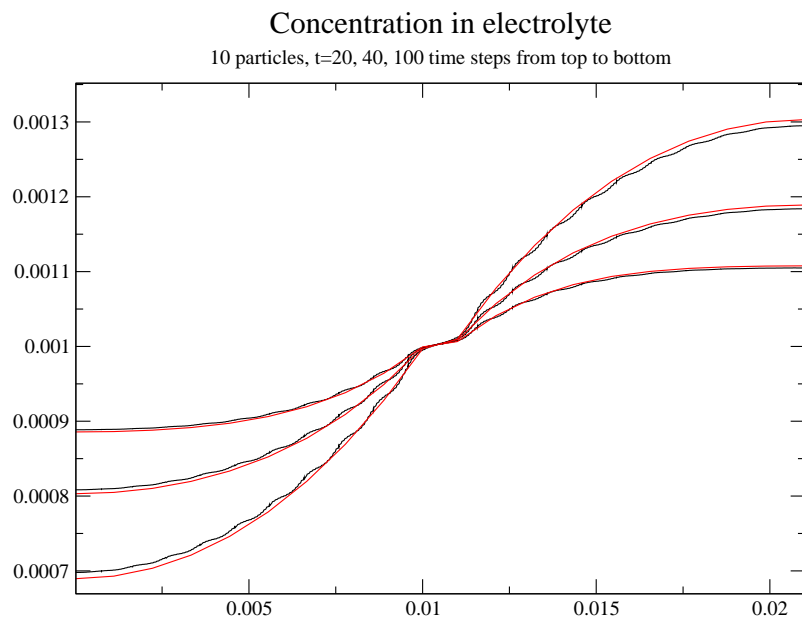


Figure 25: Comparison between the homogenized and the microscopic solution: concentration of  $\text{Li}^+$  in the electrolyte for  $10 \times 10 \times 10$  particles in each electrode for different time steps

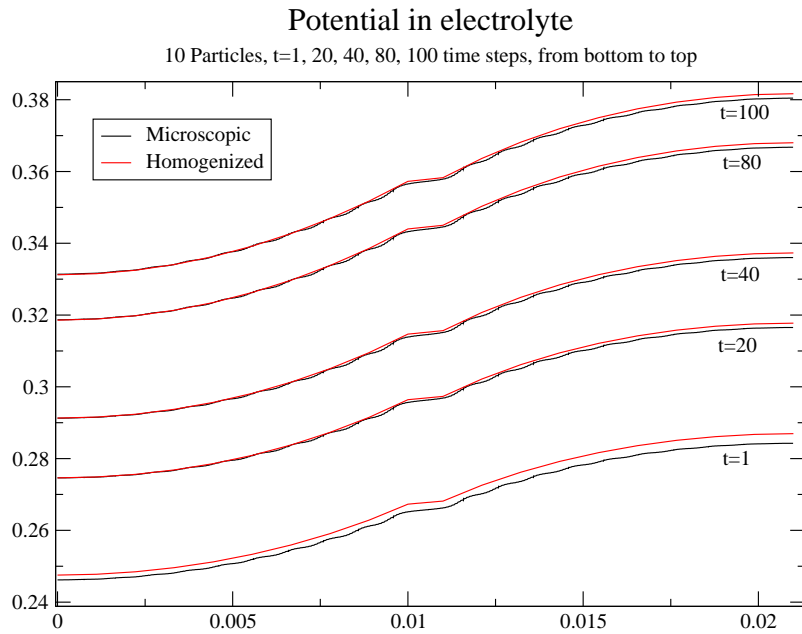


Figure 26: Comparison between the homogenized and the microscopic solution: potential in the electrolyte for  $10 \times 10 \times 10$  particles in each electrode for different time steps

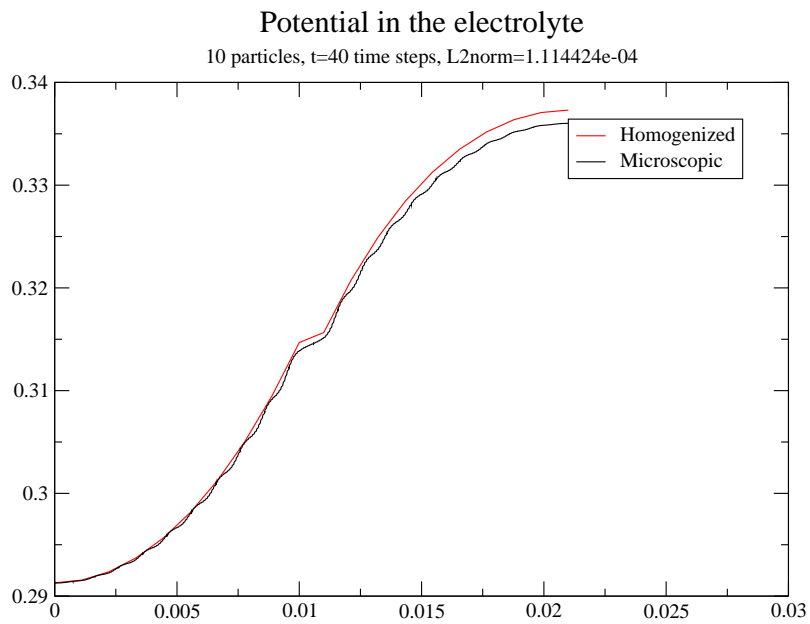


Figure 27: Comparison between the homogenized and the microscopic solution: potential in the electrolyte for  $10 \times 10 \times 10$  particles in each electrode



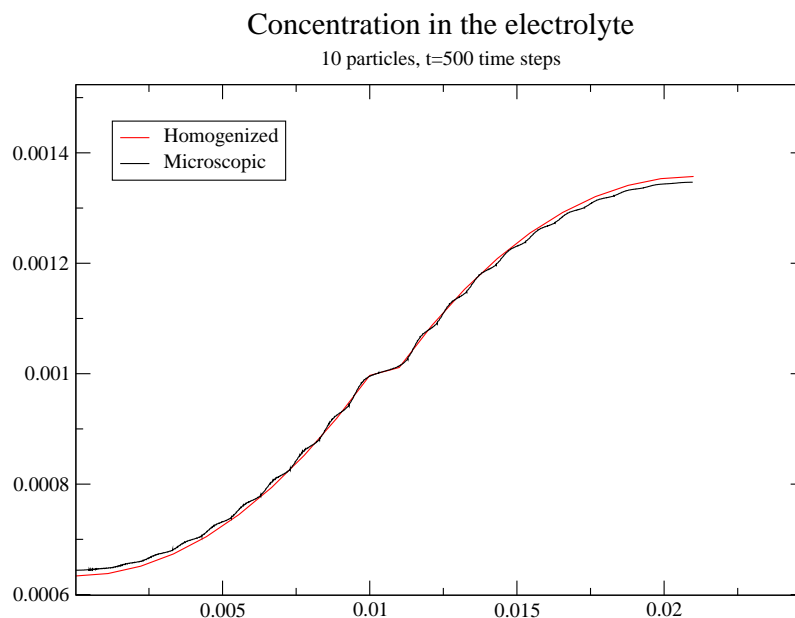


Figure 28: Concentration in the electrolyte for  $10 \times 10 \times 10$  particles in each electrode after 500 time steps,  $L_2$  norm= $1.05651e-06$

### 9.3 Experiment 3

In this experiment we run simulations for 20 active particles in each direction, which means that we have a total number of 8000 particles in each electrode. The characteristic size of the particles is  $5\mu\text{m}$  and the small parameter is  $\varepsilon = 0.05$ . The results from the full microscopic simulation and from the homogenized problem are given in Figure 29, 30, 31 and 32. In Figure 33 we show the concentration of Lithium ions in the anode after 80 time steps.

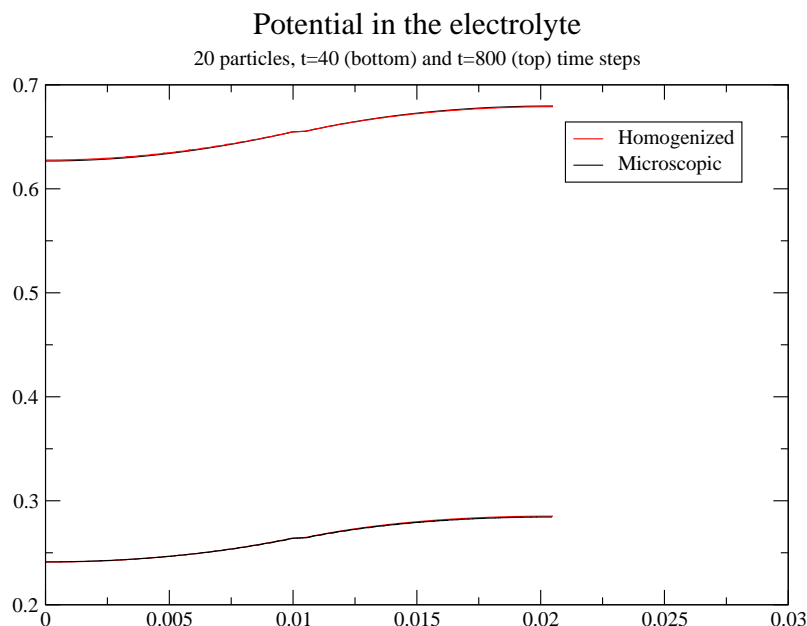


Figure 29: Comparison between the homogenized and the microscopic solution: potential in the electrolyte for  $20 \times 20 \times 20$  particles in each electrode for different time steps

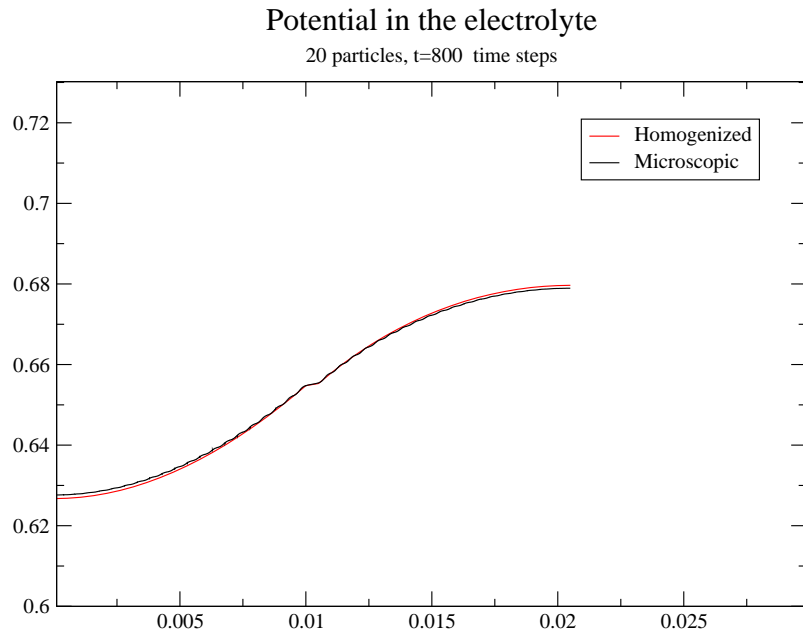


Figure 30: Comparison between the homogenized and the microscopic solution: potential in the electrolyte for  $20 \times 20 \times 20$  particles in each electrode for different time steps

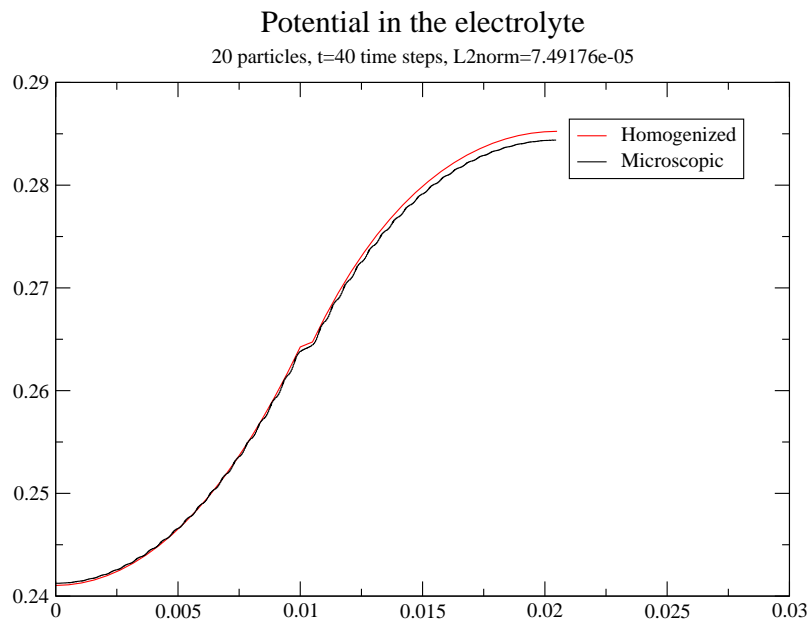


Figure 31: Comparison between the homogenized and the microscopic solution: potential in the electrolyte for  $20 \times 20 \times 20$  particles in each electrode

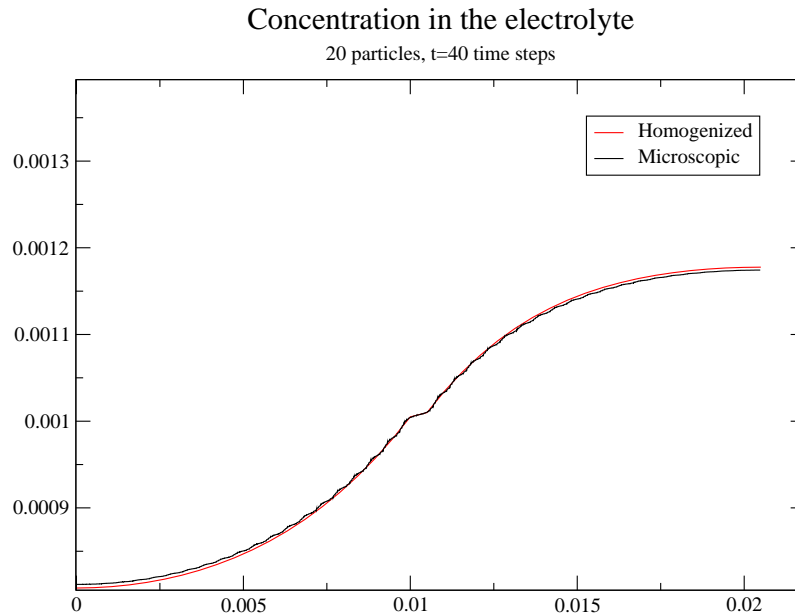


Figure 32: Comparison between the homogenized and the microscopic solution: concentration in the electrolyte for  $20 \times 20 \times 20$  particles in each electrode

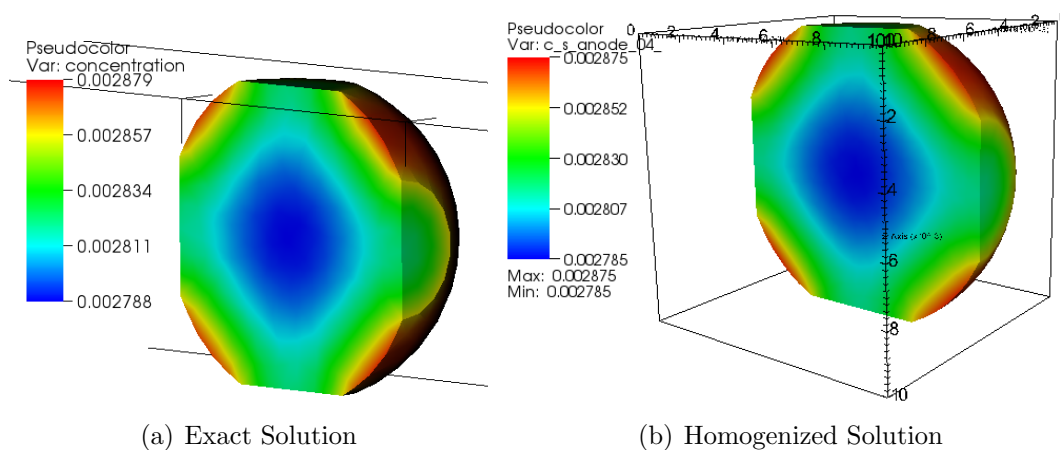


Figure 33: Concentration in the Anode after 80 time steps for 8000 particles in each electrode

## 9.4 Experiment 4

In this experiment we run simulations for 40 active particles in each direction, which means that we have a total number of 64000 particles with typical size of  $2.5\mu\text{m}$  in each electrode. Consequently we have that  $\varepsilon = 0.025$ . The results from the full microscopic simulation and from the homogenized problem are given in Figure 34 and 35.

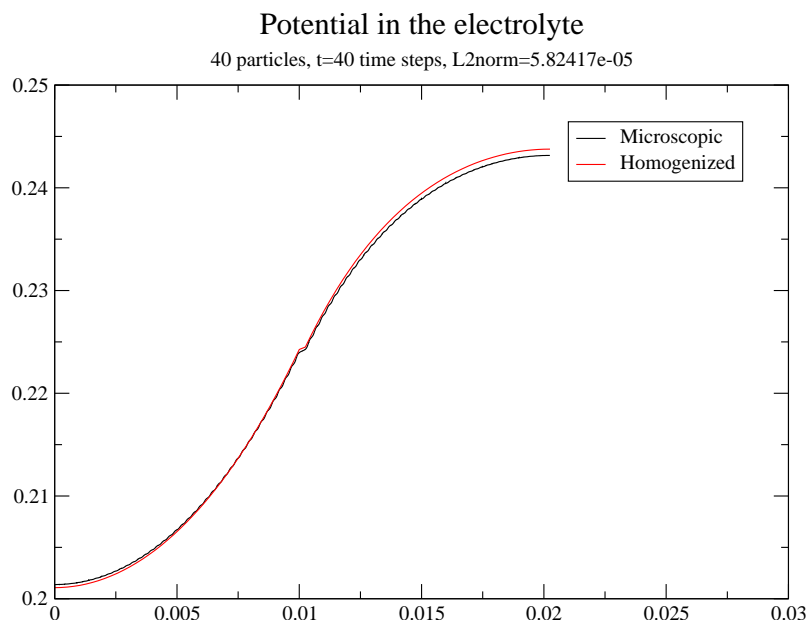


Figure 34: Comparison between the homogenized and the microscopic solution: potential in the electrolyte for  $40 \times 40 \times 40$  particles in each electrode

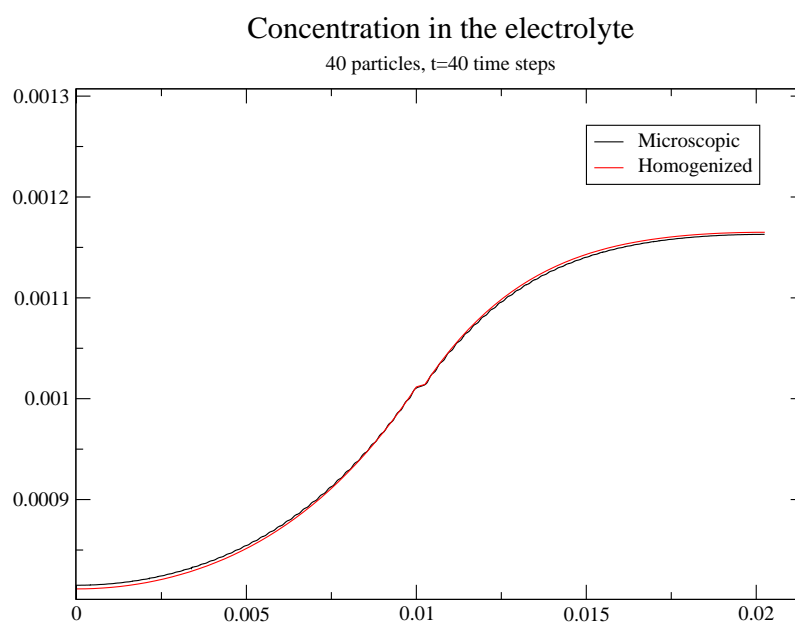


Figure 35: Comparison between the homogenized and the microscopic solution: concentration in the electrolyte for  $40 \times 40 \times 40$  particles in each electrode

## 10 Conclusion

The theoretical error estimate for linear elliptic problems is

$$\|u_\varepsilon - u_0 - \varepsilon u_1\|_{H^1(\Omega)} \leq C\sqrt{\varepsilon} \quad (10.1)$$

where  $u_\varepsilon$  is the microscopic solution,  $u_0$  is the solution of the homogenized problem and  $u_1$  is the first order corrector (see [4]). As we can see from Table 2 the  $L_2$  norm of the difference between the homogenized and the microscopic solution decreases when we decrease  $\varepsilon$ .

Table 2:  $L_2$  norm at time step 40

Particles	$\varepsilon$	$\ \phi_0^e - \phi^e\ _{L_2}$	$\ c_0^e - c^e\ _{L_2}$	$\ \phi_0^s - \phi^s\ _{L_2}$
				Cathode
5	0.2	3.76515e-04	8.73508e-07	0.000393077
10	0.1	1.114424e-04	5.60168e-07	0.000139498
20	0.05	7.49176e-05	4.41375e-07	7.30204e-05
40	0.025	5.82417e-05	3.66711e-07	3.5623e-05

We have successfully derived a coupled micro-macroscale model for the isothermal Li-ion battery model [8]. We rigorously proved the order of the current density which is crucial for the correct homogenization of the microscopic model. We also derived properly upscaled Neumann boundary conditions. Finally we ran a series of numerical simulations for uniformly decreasing  $\varepsilon$  against FEM solver for the microscopic model. The results of the simulations show good agreement between the homogenized and the microscale solutions. We should also note that the proposed solution algorithm allows for a trivial parallelization for solving the microscale problem for  $c^s$ .

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